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TOWARD A MATHEMATICAL THEORY OF ENVIRONMENTAL MONITORING: THE INFREQUENT SAMPLING PROBLEM

Kenneth D. Pimentel
(Ph. D. Thesis)

June 1975

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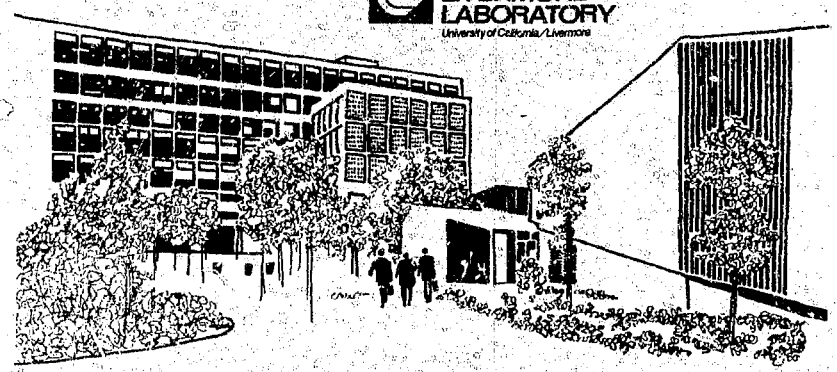

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Kenneth D. Pimentel
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ABSTRACT

An environmental monitor is taken to be a system which generates estimates of environmental pollutant levels throughout an environmental region for all times within a time interval of interest from measurement data taken only at discrete times and only at discrete locations in that region. This study addresses the following optimal environmental monitoring problem: determine the optimal monitoring program — the numbers and types of measurement devices, the locations where they are deployed and the timing of those measurements — which minimizes the total cost of taking measurements while maintaining the error in the pollutant estimate below some bound throughout the time interval of interest.

Diffusive pollutant transport in distributed environmental systems is treated with the method of separation of variables to obtain a set of stochastic first-order ordinary differential state equations for the process. Techniques of optimal estimation theory are applied to this set of state equations yielding a set of matrix estimation error covariance equations whose solutions are used in accuracy measures for the resulting estimates in the synthesis of optimal monitors.

The main results are associated with the infrequent sampling problem. If the estimation error constraints imposed upon the monitor are sufficiently lax, the solution for the optimal monitoring program results in relatively long times between required measurements. This leads to drastic simplifications in the solutions of the problems of optimally designing and sequencing the measurements, where only certain terms in the solutions of the estimation equations are found to effect the response for large time. This dominance of certain asymptotic terms is seen as a potential area for future application in more complex environmental pollutant transport problems.

Owing to the ease in their interpretation, numerical applications for one-dimensional diffusive systems are included to illustrate the main results, though all the results are shown to generalize to the three-dimensional case. Considerable use of graphical computer output is made which clearly exhibits the features of the infrequent sampling problem. An extensive list of references in areas relevant to the optimal monitoring problem completes this report.

TABLE OF CONTENTS

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The approach of the conclusion of my doctoral studies has prompted a wide variety of responses from those closest to me. From my daughter, Jennifer, who's almost five, "I missed you today". From my son, John,

who's almost three, "Daddy, don' go wurk anymoi--stay home now". And from my wife, Janet, who alone knows how old she really is, "I don't believe it". Thank you, Hunny, for always being there and yes, it *is* done. Now, where'd you want that pool?

DEDICATION

for JVP, Ph.D.

LIST OF CONCLUSIONS

NOMENCLATURE

Symbol	Description
$\underset{\sim}{A}(t)$, $\underset{\sim}{A}$	Continuous-time dynamic system matrix
$\underset{\sim}{B}(t)$, $\underset{\sim}{B}$	Continuous-time deterministic input distribution matrix
$\underset{\sim}{C}(t)$, $\underset{\sim}{C}$	Continuous-time measurement matrix
$\underset{\sim}{C}_K$	Discrete-time time-varying measurement matrix at time t_K
$\underset{\sim}{C}_K^*$	The optimal measurement matrix at time t_K
$\underset{\sim}{C}(\underset{\sim}{z}_K)$	Measurement matrix as a function of the vector $\underset{\sim}{z}_K$ of measurement positions at time t_K
C_n	Generalized modal capacitance
$\underset{\sim}{D}(t)$, $\underset{\sim}{D}$	Continuous-time stochastic disturbance distribution matrix
$\underset{\sim}{E}_{ij}$	*Unit matrix with* (i,j)*th element equal to one* and all other elements zero
F	Pollutant mixing ratio
$\underset{\sim}{G}_{K+1}$	Kalman gain matrix at time t_{K+1}
$\underset{\sim}{I}$	Identity matrix
J	Performance criterion
$J_1(t)$	First monitor performance criterion: estimation error in optimal state estimate at time t
$J_2(\underset{\sim}{\zeta}^*,t)$	Second monitor performance criterion: value of *pollutant concentration estimation error* at that point $\underset{\sim}{\zeta}^*$ in the medium where it is a maximum at time t
K	Diffusion coefficient; discrete-time index; final value of a discrete-time summation index
L, 2L	Length of a one-dimensional diffusive medium
$\underset{\sim}{M}_0$	Covariance matrix for initial state

Symbol	Description
N	Final value of a discrete-time summation index
P	Region in space over which pollutant transport problem is defined
$\underset{\sim}{P}_K^K$	Corrected state estimation error covariance matrix at time t_K conditioned upon all past measurements including the measurement at time t_K
$\underset{\sim}{P}_{K+1}^K$	Predicted state estimation error covariance matrix at time t_{K+1} conditioned upon all past measurements up to and including the measurement at time t_K
$\underset{\sim}{P}_{K+N}^K(\underset{\sim}{\zeta}_K)$	Predicted state estimation error covariance matrix at time t_{K+N} conditioned upon all past measurements up to and including the last measurement at time t_K and a function of the measurement matrix at time t_K
$\underset{\sim}{P}(t)$, $\underset{\sim}{P}$	Continuous-time state estimation error covariance matrix
R_n	Generalized modal resistance
T	Discrete-time integration step-size
Tr_{lim}	First monitoring error constraint: maximum allowable error in the estimate of the monitor state vector
$Tr\left[\underset{\sim}{P}_{K+N}^K(\underset{\sim}{z}_K^*)\right]$	Predicted value of the trace of the state estimation error covariance matrix at time t_{K+N} conditioned upon all past measurements up to and including the optimal measurement at $\underset{\sim}{z}_K^*$ at time t_K
$\underset{\sim}{V}(t)$, $\underset{\sim}{V}$	Continuous-time measurement error covariance matrix
$\underset{\sim}{W}(t)$, $\underset{\sim}{W}$	Continuous-time state disturbance covariance matrix
$\underset{\sim}{X}$	A matrix used in derivations
$\underset{\sim}{Y}$	A matrix used in derivations
c	Scalar measurement coefficient used in optimal management problem derivations
$\underset{\sim}{c}(\underset{\sim}{\zeta})$, $\underset{\sim}{c}$	Readout vector mapping modal states into pollutant concentration at point $\underset{\sim}{\zeta}$ in space

Symbol	Description
e	Base of natural logarithms (= 2.71828 ...); surface emissivity coefficient
$e^{\underset{\sim}{A}T}$	Exponential of the matrix $[\underset{\sim}{A}T]$
$\underset{\sim}{e}_i$	Unit vector with ith element equal to one and all other elements zero
$e_n(z)$	Eigenfunction associated with the nth eigenvalue evaluated at position z
f	Stochastic pollutant source term in the transport equations
g	Deterministic pollutant source term in the transport equations
h	Emission boundary condition coefficient
i	Vector or matrix element index
j	Vector or matrix element index
m	The dimension of the noise-corrupted measurement, measurement error and measurement position vectors $\underset{\sim}{y}_K$, $\underset{\sim}{v}_K$, and $\underset{\sim}{z}_K$
$\underset{\sim}{m}_0$	Mean value of initial state
n	Discrete-time summation index
n	The dimension of the state and optimal state estimate vectors $\underset{\sim}{x}_K$ and $\hat{\underset{\sim}{x}}_K$
p	Scalar state estimation variance used in optimal management problem derivations
p	The dimension of the deterministic input vector $\underset{\sim}{u}(t)$
r	The dimension of the stochastic state disturbance vector $\underset{\sim}{w}(t)$
t	Continuous value of time
t_K	The Kth discrete value of time
$\tilde{\underset{\sim}{u}}_K$	Convolution of deterministic input vector over the time interval $[t_K, t_{K+1}]$

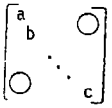
Symbol	Description
$\underset{\sim}{u}(t)$, $\underset{\sim}{u}$	Continuous-time deterministic input vector
$\underset{\sim}{v}_K$	Discrete-time measurement error vector at time t_K
$\underset{\sim}{v}(t)$, $\underset{\sim}{v}$	Continuous-time measurement error vector
$\tilde{\underset{\sim}{w}}_{K+1}$	Convolution of the stochastic disturbance vector over the time interval $[t_K, t_{K+1}]$
$\underset{\sim}{w}(t)$, $\underset{\sim}{w}$	Continuous-time stochastic disturbance vector
$\dot{\underset{\sim}{x}}$	Derivative with respect to time of the state vector $\underset{\sim}{x}$
$\underset{\sim}{x}_K$	Discrete-time state vector at time t_K
$\hat{\underset{\sim}{x}}_K^K$	Corrected value of the optimal state estimate at time t_K conditioned upon all past measurements including the measurement at time t_K
$\hat{\underset{\sim}{x}}_{K+1}^K$	Predicted value of the optimal state estimate at time t_{K+1} conditioned upon all past measurements up to and including the measurement at time t_K
$\underset{\sim}{x}(t)$, $\underset{\sim}{x}$	Continuous-time state vector
$\hat{\underset{\sim}{x}}(t)$, $\hat{\underset{\sim}{x}}$	Optimal estimate of continuous-time state vector
$\underset{\sim}{y}_K$	Discrete-time noise-corrupted measurement vector at time t_K
$\underset{\sim}{y}(t)$, $\underset{\sim}{y}$	Continuous-time, noise-corrupted measurement vector
z	Position in a one-dimensional diffusive medium
z^*	Position of maximum error (variance) in the estimate of the pollutant concentration over all values of z in a one-dimensional medium
$\underset{\sim}{z}_K$	Discrete-time measurement position vector at time t_K
$\underset{\sim}{z}_K^*$	Vector of optimal measurement positions at time t_K
$\underset{\sim}{z}_u$	Vector of deterministic input point source locations

Symbol	Description
$\underline{z}_w$	Vector of stochastic disturbance point source locations
$\underline{0}$, $\underline{o}$	Zero matrix or vector
α	Pollutant scavenging parameter
$\underline{\Gamma}_{K+1}$ $\underline{\Gamma}$	Time-invariant discrete-time stochastic disturbance distribution convolution matrix for the fixed time step $T \equiv (t_{K+1} - t_K)$
Δ_K	Amount of correction to scalar state estimation variance for a measurement at time t_K used in the optimal management problem derivations
ΔTr_K	Amount of correction to the trace of the state estimation error covariance matrix for a measurement at time t_K used in the optimal management problem derivations
$\delta(t-\tau)$	Dirac delta function
δ_{Kj}	Kronecker delta function
ε	A convergence criterion
$\underline{\zeta}$	Position coordinate vector for a point in a region P in a diffusive medium
η	An intermediate transformation variable
$\underline{\Theta}$	A matrix used in certain derivations
λ_n	Eigenvalue or separation constant
μ_n	Terms involved in determination of eigenvalues for emission boundary conditions
$\xi(\underline{\zeta},t)$, ξ	Pollutant concentration at point $\underline{\zeta}$ in space at time t
$\hat{\xi}(\underline{\zeta},t)$, $\hat{\xi}$	Optimal estimate of pollutant concentration at point $\underline{\zeta}$ in space at time t
$\xi_K(z)$, ξ_K	Discrete-time pollutant concentration at point z and time t_K

Symbol	Description
$\hat{\xi}_K(z)$, $\hat{\xi}_K$	Optimal estimate of discrete-time pollutant concentration at point z and time t_K
$\xi_0(z)$	Initial pollutant concentration as a function of position z in the medium
π	= 3.14159...
ρ_{ij}^N	A convergence measure
$\sigma^2(\underline{\zeta},t)$	Variance in the optimal continuous-time estimate of pollutant concentration at point $\underline{\zeta}$ in space at time t
$\sigma_K^2(z)$	Variance in the optimal discrete-time estimate of the pollutant concentration at point z and time t_K
$\sigma_{K+N}^2(\underline{z}_K,z)$	Predicted value of the variance at time t_{K+N} in the discrete-time estimate of the pollution concentration at point z conditioned upon measurements up to and including the last measurement with position vector $\underline{z}_K$ at time t_K
$\sigma_{K+N}^2(\underline{z}_K^*,z^*)$	Predicted value of the maximum value over all values of z of the variance in the pollutant concentration at time t_{K+N} conditioned upon all past measurements up to and including the optimal measurements at $\underline{z}_K^*$ at time t_K
$\sigma_K^2(\underline{z}_K^*,z^*)$	Corrected value of the maximum value over all values of z of the variance in the pollutant concentration at time t_K conditioned upon all past measurements including the optimal measurements at $\underline{z}_K^*$ at time t_K
σ_{lim}^2	Second monitoring error constraint: maximum allowable error in the estimate of the pollutant concentration anywhere in the medium
τ	Time, used in certain definitions and derivations
$\underline{T}$	An intermediate matrix used in various derivations
ν	Scalar measurement error variance used in optimal management problem derivations

Symbol	Description
$\underset{\sim}{\Phi}_{K+1}^{K}$, $\underset{\sim}{\Phi}$	Time-invariant state transition matrix for the fixed time step $T \equiv (t_{K+1} - t_K)$
$\underset{\sim}{\Phi}(t_{K+1},t_K)$	Time-varying state transition matrix between times t_K and t_{K+1}
$\underset{\sim}{X}$	A matrix used in certain derivations
$\underset{\sim}{\Psi}_{K+1}^{K}$, $\underset{\sim}{\Psi}$	Time-invariant discrete-time deterministic input distribution convolution matrix for the fixed time step $T \equiv (t_{K+1} - t_K)$
$\underset{\sim}{\Omega}_{K+1}$, $\underset{\sim}{\Omega}$	Discrete-time convolution of the continuous-time state disturbance covariance matrix $\underset{\sim}{W}(t)$ over the interval $[t_K,t_{K+1}]$
$\underset{\sim}{\Omega}_{N}$	The discrete-time matrix convolution of the matrix $\underset{\sim}{\Omega}_{K+1}$ where N terms in the series are included
$\underset{\sim}{\Omega}_{SS}$	The limit of the discrete-time matrix convolution $\underset{\sim}{\Omega}_{N}$ as N approaches infinity with its (1,1)-element set to zero
ω	Scalar state disturbance variance used in optimal management problem derivations
$\approx$	Approximately equals
$\equiv$	Identically equals or is defined as
$>$	Greater than
$>>$	Much greater than
$<$	Less than
$\leq$	Less than or equal to
$\propto$	Proportional to or goes like
$\rightarrow$	Approaches or goes to
$\Rightarrow$	Implies or infers
$d[\cdot]$	Total differential operator
$\frac{d}{dt}[\cdot]$, $[\dot{\cdot}]$	Derivative with respect to time of the variable in brackets

Symbol	Description
$\frac{\partial}{\partial c}$	Partial differentiation of a variable with respect to the scalar c
$\frac{\partial}{\partial \underset{\sim}{c}}$	Partial differentiation of a variable with respect to the vector $\underset{\sim}{c}$
$\frac{\partial}{\partial \underset{\sim}{\underset{\sim}{C}}}$	Partial differentiation of a variable with respect to the matrix $\underset{\sim}{\underset{\sim}{C}}$
$diag\ [\cdot]$	A vector whose elements are the diagonal elements of the matrix enclosed in brackets
$E[\cdot]$	Expectation operator for a random variable, vector or matrix
$\lim_{N\to\infty}$	Limiting operation as N approaches infinity
$\max_{z}$	Maximum over all scalar values of z
$\min_{\underset{\sim}{z}_K}$	Minimum over all vector values of $\underset{\sim}{z}_K$
$\min_{\underset{\sim}{z}_K} \max_{z}$	Simultaneous *minimum* over all vector values $\underset{\sim}{z}_K$ and maximum over all scalar values z
$\sum_{n=1}^{N}$	Summation from 1 to N over all values of the index n
$Tr[\cdot]$	Trace operator of the matrix enclosed in brackets
$[\cdot]_i$	The i<u>th</u> element of the vector enclosed in brackets; $[\underset{\sim}{a}]_i$ is also denoted a_i
$[\cdot]_{ij}$	The (i,j)th element of the matrix enclosed in brackets; $[\underset{\sim}{\underset{\sim}{A}}]_{ij}$ is also denoted A_{ij}
$[\cdot]^T$	Transpose operation for a vector or matrix
$[\cdot]^{-1}$	Inverse operation for matrices
$\begin{bmatrix} a & \\ & \underset{\sim}{\underset{\sim}{O}} \end{bmatrix}$	A matrix with (1,1)-element equal to a and all other elements zero
$\begin{bmatrix} 0 & \\ & \underset{\sim}{\underset{\sim}{A}} \end{bmatrix}$	A matrix with (1,1)-element equal to zero and all other elements equal to the elements of the matrix $\underset{\sim}{\underset{\sim}{A}}$

Symbol	Description
	A diagonal matrix
$\underset{\sim}{P} > 0$	The matrix $\underset{\sim}{P}$ is positive definitive
∞	Infinity

CHAPTER 1. INTRODUCTION

The problem of the optimal monitoring of pollutants in environmental systems concerns the minimum cost estimation of pollutant levels throughout a region while maintaining the errors in the estimates within a given bound. The optimal monitor synthesis problem considered in this thesis logically separates into the two monitoring subproblems of optimal design and optimal management. Optimal monitoring system design includes the specification of a model for the physical system, the choice of measured variables, measurement devices and their spatial distribution in the medium. The optimal management problem concerns finding the best sequencing of measurements in time to result in the minimum cost sampling program. The optimal monitor is then defined as that solution of the design and management problems together which results in the minimum cost measurement program necessary to maintain the error in the pollutant estimate below a given bound over the time interval of interest.

This is a departure from most studies in the optimization of systems with cost for observation in that use is not made of a combined performance criterion which typically consists of the time integral of a weighted combination of measurement cost and estimation error. Instead, in this study, advantage is taken of the separation of the design and management problems whose two solutions separately determine the characteristics of the measurements at the required sample times, and the timing of those measurements themselves. Thus, estimation error is not minimized, but rather, bounded in a

fashion which corresponds with actual applications where legal limits are placed upon allowable errors in the pollutant level estimates in environmental monitors. It is bounded in such a manner that the minimum total number of samples is necessary over some time interval, resulting in the minimum cost monitoring program.

The separation of the monitoring design and management problems was proposed by Brewer and Moore [24]. Moore [95] has considered application of such concepts to the area of aquatic ecosystems, where the Extended Kalman Filter is applied to the highly nonlinear equations of the dynamics of population growth of aquatic constituents. This thesis, instead, concentrates upon strictly linear processes in the hope that the mathematical simplifications possible there may be extendable to the nonlinear case in future studies. In the optimal estimation of the state vector of a linear, discrete-time, stochastic system, the Kalman Filter [66] provides a particularly elegant computational solution. The two equations for prediction and correction of the associated state estimation error covariance matrix have been conjectured by Brewer and Moore [24] as containing the key to the solution of the management problem; it is shown here that they indeed do lead to a problem structure which results in the optimal solution of not only the management problem, but to that of the design problem as well.

Owing to the anticipated complexities of the optimizations associated with the various parts of the monitoring problem, advantage is taken of the simplicity of the separation of variables technique in the theory of linear, partial differential equations in obtaining ordinary differential equation models for distributed systems (see Berg

and McGregor [18]). In reducing the resulting state spaces for such normal mode models to spaces of finite dimension, the quantitative methods recently developed by Young [131] in atmospheric modeling greatly extend the area of applicability of such analytical techniques. In particular, nonhomogeneous, anisotropic media may be handled by the spatial discretization of the medium into component subregions over which constant average values for system parameters are sufficiently accurate. Component coupling by the use of pseudo-sources to make up for differences in the normal mode submodels is the key factor given by Young which allows for the simple approximation of the dynamic response of large, varied, distributed environmental systems. The existence of these techniques underlies the studies in this thesis in their extension to large scale practical problems in environmental monitoring.

With the use of a finite-dimensional, normal mode state model, the resultant continuous-time state equations are discretized in time for use in the Kalman Filter. The nature of the Kalman Filter is now well known in its applications in the aerospace field. Recent applications in more diverse areas (see, for example, the special issue in IEEE [62]) have established it as a powerful tool of broad scope in the field of system estimation. Its numerical advantages over other optimal estimation techniques (well documented in Gelb [44]) make it the logical choice for use in environmental monitoring systems where processes of interest may dictate the use of huge models to obtain desired levels of spatial and temporal resolution in the results.

The main results of this thesis concern the special class of monitor addressed in the infrequent sampling problem. This case is characterized by high levels of allowable pollutant estimation error which result in relatively long periods between required sample times. These long times between samples allow the transient terms involved in the growth of the uncertainty in the pollutant estimates to reach steady-state values so that only asymptotic solutions of the estimation error covariance equations need be considered in the design and management problems. This drastically simplifies the solution of the monitoring problem for the case of infrequent sampling.

Applications of the theory developed here are seen to arise in any environmental or other dispersive system where the dynamics of the dispersal of the pollutant or variable involved is dominated by diffusion and where convective transport can be ignored. This rules out its use in air quality monitoring systems on a regional basis where convection typically dominates diffusion in pollutant transport by a ratio of 30:1 [76]. However, as developed by others cited in Young [131], models of pollutant transport on a global scale are often based upon diffusion as the dominant mechanism of dispersal. In fact, examples in Young indicate that the normal mode modeling techniques mentioned earlier can be successfully applied to global atmospheric modeling where only diffusion is included as the dispersion mechanism.

An interesting extension of the results of this thesis might be to a study involving assessment of the climatic impact of flying a fleet of SST's upon the protective ozone layer in the atmosphere (see, for example, Mac Cracken, *et al.* [80]). In such an application, knowing where and when to best sample atmospheric pollutant levels could greatly

facilitate validation of numerical atmospheric models, in initial applications, and greatly reduce long-range monitoring costs upon implementation of such a program.

Groundwater systems seem to be a probable area of application, as indicated in what follows, though no experimental verifications have been attempted. Systems involving heat transfer by conduction which involve stochastic heat sources could find application for the theory of the infrequent sampling problem. For example, in nuclear reactor cooling systems, a central control computer could be time-shared to consider only the best sites for temperature measurement in the walls of the pressure vessel over time.

The need for better environmental monitoring has been described in the literature [46,95,102]; typical measurement costs have been tabulated [14]. Propagation of uncertainty in distributed systems has been considered in some detail [56,59,101]. Related studies using other approaches do not address the monitoring problem either as it separates into the design and management problems, or with the drastic simplifications which arise in the infrequent sampling problem (see the work of Seinfeld [113], Seinfeld and Chen [114,115], Seinfeld and Lapidus [116], Reiquam [104], Bensoussan [17], Soeda and Ishihara [119]). Thus, there is a need for improvement of the synthesis procedures for monitoring systems in large scale environmental problems.

The thesis is organized into seven chapters and seven appendices, to keep things even. Chapter 2 summarizes work by others in germane problem areas and defines the scope of the present study. Chapter 3 develops briefly the normal mode modeling technique of the application of the method of separation of variables. Chapter 4 deals with the

time-discretization of the associated finite set of continuous-time, ordinary differential state equations and summarizes the more salient features of Kalman Filter Theory. Chapter 5 presents the main theory associated with the infrequent sampling problem, punctuated with conclusions as they can be made. Application and demonstration of the analytical results of Chapter 5 are made in the numerical examples of Chapter 6, in which more conclusions are seen to follow. In Chapter 7, the main results for the optimal monitoring problem for the case of infrequent sampling are collected in summary and possible extensions for future study indicated. Some of the more routine analytical developments, as well as all of the computer program listings, are gathered in the appendices. A rather extensive list of references relevant to the optimal estimation, monitoring and measurement system design problems completes this document.

CHAPTER 2. BACKGROUND AND PROBLEM STATEMENT

This chapter begins with a summary of representative work done by others in fields of importance to the environmental monitoring problem. An attempt is made to present a reasonably complete survey of pertinent literature in the hope that future researchers may benefit from the sources this author has utilized.

The broad area of optimal measurement system design is then narrowed greatly in scope as it applies to problems in certain classes of environmental pollutant transport. The problems of the optimal design and management of environmental quality monitoring systems are finally stated in the contexts of two cases for bound on the allowable error in either the monitor state or the monitor output estimate.

2.1 Background

The major topics of concern in the study of environmental monitoring systems in this thesis include the following: mathematical modeling in dispersive environmental systems; the numerical treatment of certain classes of partial differential equations; the stability and asymptotic solutions of systems of ordinary differential equations; optimization of a function of several variables; deterministic dynamical system theory; stochastic system theory and optimal estimation; optimal measurement system design in lumped and distributed parameter systems and finally, monitoring system synthesis for environmental applications.

Considerable interest has been turned to problems in the dispersal of pollutants in environmental systems in recent years. Some typical contributions in the areas of the atmospheric sciences include the modeling of air pollutant transport on a regional basis [81], the climatic

impact of flying a fleet of SST's in the upper atmosphere [80], studies in the parameter sensitivity of models of the planetary boundary layer [35,99], and studies of models of the global transport of pollutants [36,131]. In one recent study by Young [131], the classical methods of applied mathematics were successfully applied to the solution of global pollutant transport problems in a unique way that takes advantage of analytical results available for certain classes of partial differential equations. By the expansion of solutions for such equations in infinite series form, followed by quantitatively meaningful truncation of those serious solutions, approximate solutions for otherwise large, difficult problems can be obtained. This procedure involves coupling together solutions for problems in adjacent subregions to efficiently approximate the response in larger areas. The theory for such Fourier-type expansions is now well established [18,34,82,118] but the unique extensions made by Young possess the potential for applying classical normal-mode analysis long associated with problems in the mechanics of linear solids [93,47] to a far broader class of problems, including environmental pollutant transport in nonhomogeneous, anisotropic media.

This author follows Young in the application of normal-mode techniques to problems in the solution of the dynamic equations of environmental pollutant transport. Such methods yield finite sets of ordinary differential equations whose solutions form time-varying multipliers for the spatial mode shapes which comprise the normal mode solution; bond graphs are seen to offer a concise graphical representation of such normal mode models (see, for example, Karnopp and Rosenberg [69]). The study of the numerical treatment of systems of ordinary differential equations is a fundamental part of the solution of the monitoring problem when using

the normal mode approach; recent advances in the numerical solution of general, nonlinear, time-varying, possibly stiff, ordinary differential equations are typified by the work of Gear [43], Hindmarsh [57,58], and Byrne and Hindmarsh [25]. Analytical treatments can be found in Coppel [28].

In the case of linear, time-invariant ordinary differential equations, the class involved in the infrequent sampling problem considered in this study, the powerful techniques of linear system theory can be used (see, for example, Desoer [32], Takahashi, *et al.* [121], Brewer [22], Freeman [41], Timothy and Bona [123],and Schultz and Melsa [109]). In the actual implementation of algorithms associated with the solutions of such linear systems, certain topics in matrix theory in numerical analysis prove to be useful [38,40,129]. Involved in the optimal design problem in monitoring system synthesis are the problems associated with the optimization of a function of several variables; Beveridge and Schechter [20] is found to be an excellent reference in this area, while Fleming [37] provides a more firm background in the theory of a function of several variables. A gradient routine by Westley [127] was chosen for the constrained minimization of the nonlinear objective functions associated with the optimal design problem. Such gradient methods are contrasted, for example, with the work of Radcliffe and Comfort [103] in which constrained direct search methods are presented which do not involve the use of derivatives of the objective function; gradient methods are found to offer computational advantages over direct search methods in their application to the optimizations involved in the optimal design problem. In the particular problems of finding the position of maximum uncertainty in the pollutant estimate for the monitoring problem with

bound on error in the output estimate, root finding methods for finding zeros in the derivative of the expression for the error were found to be superior to direct search methods for such scalar maximizations (see Hausman [53,54]).

The field of optimal state estimation in stochastic dynamic system theory is well developed in what it offers for the solution of the optimal monitoring problem. Gelb [44,122] makes a particularly lucid presentation of the more practical topics in applied estimation theory; the original work of Kalman [66] and Kalman and Bucy [67] still stand as basic reference material for the concepts involved. Sorensen (in Leondes [78]) presents a concise introduction to Kalman filter techniques; Meditch [85] also presents a clear development of the optimal filter. Aoki [3] contains a considerable amount of material concerned with special topics in stochastic system theory, as does Sage [105]. Jazwinski [65] is sufficiently complete in its rigor to serve as one single reference in the area of stochastic processes and filtering theory; for more fundamental material in the theory of stochastic differential equations, including a particularly rigorous development of the Kalman-Bucy Filter, see Arnold [6].

The Special Issue of IEEE Transactions on Automatic Control, December 1971, dealing with the Linear-Quadratic Gaussian Problem [62], offers an extensive collection of topics in optimal estimation theory; it includes a well edited bibliography which should be a basic resource to any researcher in this field. The proceedings of a special conference sponsored by NATO [98] summarizes many military and aerospace applications of estimation theory.

There are many special topics in estimation theory which could prove of importance in future extensions of the work in this thesis to practical applications in nonlinear systems. Of them, adaptive filtering is of particular importance; see the work of Mehra [86,87,88,89], Jazwinski [64], Berkovec [19], Godbole [45], Nahi and Weiss [97], and Scharf and Alspach [108]. Extensions to nonlinear estimation are considered in Wishner, *et al.*[130], Athans, *et al.* [9], Wells [126], Gura [49], and Gura and Hendrikson [52]; Moore uses the Extended Kalman Filter, as cited earlier, in his work on the monitoring problem [95]. As well as Moore, others have examined the effects of using an imprecise model in the optimal filter upon the performance of optimal estimation schemes; among them are Jazwinski [65] who considers the area of filter divergence at length, Aoki and Huddle [4], Leondes and Novak [77] and Inglehart and Leondes [63].

The area of theory most closely allied to that of the optimal monitoring problem is known variously as optimal estimation with cost for observation, optimal measurement system or subsystem control or the optimal timing of measurements. Aoki and Li [5] were among the first to address such problems, along with Meier [90,91,92]. Athans uses his Matrix Minimum Principle [8] along with the work of Schweppe [11] in an application in continuous-time systems; this work is strongly based upon direct extensions of optimal control theory (see Bryson and Ho [26] or Athans and Falb [10]). Schweppe [12,110,111] has made developments of optimal measurement strategies in radar applications. Denham and Speyer [30] did some early work in midcourse guidance. Kramer and Athans [73, 74] have made recent rigorous contributions to the mathematics associated with the combined optimal control and measurement problems, along with Pliska [100].

Other studies involving the optimal timing and use of measurement data include Kushner [75], Breazeale and Jones [21], Sano and Terao [106], Hsia [60], and Dreyfus [70].

Some of the most germane references found in the area of optimal measurement system design include Cooper and Nahi [27], Sauer and Melsa [107], Vande Linde and Lavi [125], Herring and Melsa [55], Shoemaker and Lamont [117], and Soeda and Ishihara [119].

Studies which concentrate on monitoring and measurement system optimization in distributed parameter systems include the work of Seinfeld [112,113,114,115,116], Draper and Hunter [33], Reiquam [104], Bensoussan [17], Atre and Lamba [13], Murray-Lasso [96], and Prado [101].

Bar-Shalom, *et al.* [15] consider monitoring systems much like those considered here but for a far more general class of problem. Moore [95] and Brewer and Moore [24] serve as the inspirational basis for much of what is developed in this thesis.

2.2 Problem Statement

Consider a region into which pollutants are being injected by a collection of deterministic and stochastic point sources. Two problems in the monitoring of the pollutant levels in that region over time are considered in this study.

First, suppose that measurements are required of pollutant levels for the purpose of closed-loop control, in which case feedback signals are to be constructed to control some of the amounts of pollutant being emitted into the medium. An example might be thermal pollution near a power station where it is required to optimally monitor temperatures in the surrounding area for the purpose of closed-loop control of the mean

power level. Assuming that a model can be constructed for the dynamics of the pollutant dispersal in the form of a finite set of first-order ordinary differential equations, whose solution forms the "state" vector for the model of the process (see Desoer [32]), it is well known that the mean square length of the error between the state vector and the estimate of the stochastic state vector is given by the trace of the estimation error covariance matrix for such a stochastic process as a function of time (see Kalman [66]). Thus, if it is required to minimize the mean square error in the estimate of the stochastic state vector, a suitable choice for the performance criterion for the optimal monitor with bound on maximum allowable error in the state estimate is

$$J_1(t) \equiv \mathrm{Tr}\left[\underline{P}(t)\right], \tag{2.1}$$

where

$$\underline{P}(t) \equiv E\left[\left(\hat{\underline{x}}(t) - \underline{x}(t)\right)\left(\hat{\underline{x}}(t) - \underline{x}(t)\right)^T\right] \tag{2.2}$$

is the estimation error covariance matrix for the optimal estimate $\hat{\underline{x}}(t)$ of the state $\underline{x}(t)$, both of dimension n, at time t, $E[\cdot]$ denotes the expectation operator applied to the random argument and $(\cdot)^T$ denotes the transpose operation. Here,

$$\mathrm{Tr}[\underline{A}] \equiv \sum_{n=1}^{n} [\underline{A}]_{ii} \tag{2.3}$$

is the trace function. The notation $[\underline{A}]_{ij}$ means the (i,j)th element of the matrix $\underline{A}$.

Second, suppose legal limits are placed upon the maximum error in the estimate of the pollutant level itself allowable at any time, anywhere in the medium. This case represents a problem of practical interest where a monitor might be used on-line to detect infractions of legal pollutant concentration levels in some airshed or watershed.

Let the concentration of a pollutant of interest as a function of space and time be denoted by $\xi(\underset{\sim}{\zeta},t)$. Define

$$\xi(\underset{\sim}{\zeta},t) \equiv \underset{\sim}{c}(\underset{\sim}{\zeta})^T \underset{\sim}{x}(t) \tag{2.4}$$

where $\underset{\sim}{x}(t)$, as before, is the state vector of dimension n of pollutant dispersal in the region, $\underset{\sim}{\zeta}$ is the coordinate position vector of the point where the concentration ξ is being calculated and where $\underset{\sim}{c}(\underset{\sim}{\zeta})$ is a vector (typically of eigenfunctions in the spatial coordinates $\underset{\sim}{\zeta}$ for the case of normal mode models) which maps the state $\underset{\sim}{x}$ into the concentration ξ at the point $\underset{\sim}{\zeta}$. In this application, the function of the monitor is to provide an estimate $\hat{\xi}(\underset{\sim}{\zeta},t)$ of $\xi(\underset{\sim}{\zeta},t)$ such that the maximum error between the pollutant concentration and its estimate is maintained below a given constraint or bound for all times of interest and throughout the medium spanned by $\underset{\sim}{\zeta}$. Thus, a measure of the uncertainty or error in the estimate of the pollutant level at some point $\underset{\sim}{\zeta}$ anywhere in the medium is given by the variance in the estimate $\hat{\xi}(\underset{\sim}{\zeta},t)$, denoted by $\sigma^2(\underset{\sim}{\zeta},t)$. Derive using (2.2),

$$\begin{aligned}
\sigma^2(\underset{\sim}{\zeta},t) &\equiv E\left[\left(\hat{\xi}(\underset{\sim}{\zeta},t) - \xi(\underset{\sim}{\zeta},t)\right)^2\right] \\
&= E\left[\left\{\underset{\sim}{c}(\underset{\sim}{\zeta})^T\left(\hat{\underset{\sim}{x}}(t) - \underset{\sim}{x}(t)\right)\right\}\left\{\underset{\sim}{c}(\underset{\sim}{\zeta})^T\left(\hat{\underset{\sim}{x}}(t) - \underset{\sim}{x}(t)\right)\right\}^T\right] \\
&= E\left[\underset{\sim}{c}(\underset{\sim}{\zeta})^T\left(\hat{\underset{\sim}{x}}(t) - \underset{\sim}{x}(t)\right)\left(\hat{\underset{\sim}{x}}(t) - \underset{\sim}{x}(t)\right)^T\underset{\sim}{c}(\underset{\sim}{\zeta})\right] \\
&= \underset{\sim}{c}(\underset{\sim}{\zeta})^T E\left[\left(\hat{\underset{\sim}{x}}(t) - \underset{\sim}{x}(t)\right)\left(\hat{\underset{\sim}{x}}(t) - \underset{\sim}{x}(t)\right)^T\right]\underset{\sim}{c}(\underset{\sim}{\zeta}) \\
&\equiv \underset{\sim}{c}(\underset{\sim}{\zeta})^T\underset{\sim}{P}(t)\underset{\sim}{c}(\underset{\sim}{\zeta}).
\end{aligned} \tag{2.5}$$

Thus, the variance in the estimate of the pollutant concentration itself, also termed the monitor output, anywhere in the medium can be expressed directly in terms of the monitor state estimation error covariance matrix $\underset{\sim}{P}(t)$ and the readout vector $\underset{\sim}{c}(\underset{\sim}{\zeta})$. Hence, a logical choice for a

performance criterion for the monitoring problem with bound on maximum allowable error in the output estimate is

$$\begin{aligned} J_2(\underset{\sim}{\xi}^*,t) &\equiv \sigma^2(\underset{\sim}{\xi}^*,t) \\ &= \max_{\underset{\sim}{\xi}} \sigma^2(\underset{\sim}{\xi},t) \\ &= \max_{\underset{\sim}{\xi}} \ \underset{\sim}{c}(\underset{\sim}{\xi})^T \underset{\sim}{P}(t) \underset{\sim}{c}(\underset{\sim}{\xi}) \\ &= \underset{\sim}{c}(\underset{\sim}{\xi}^*)^T \underset{\sim}{P}(t) \underset{\sim}{c}(\underset{\sim}{\xi}^*), \end{aligned} \tag{2.6}$$

where $\underset{\sim}{\xi}^*$ is the position of maximum variance in the estimate of the pollutant concentration, or output, at time t.

Thus, the two estimation error criteria to be considered here are given in (2.1) and (2.6) for the optimal monitoring problems with bound on state and output estimation error. Once an error criterion is selected in a given problem, the requirements of the optimal monitoring system design problem are to select the optimal choice of monitor model complexity, the optimal number and quality of measurement devices to deploy and their optimal locations in the environmental medium for all measurement times t_K over the time interval of interest. The added requirement of the problem of optimal monitoring management is to select the optimal measurement times t_K such that, together with the results for the optimal design problem, the minimum cost monitoring program is found which maintains the chosen estimation error criterion within its bound throughout the time interval of interest.

This is a somewhat different approach from those taken in the optimal design of systems with measurement cost by previous authors. Athans [7] defines a scalar cost functional which is a linear combination of the total observation cost and the mean square error in the estimate of the variables of interest. As in all problems with such combined performance

criteria, most of which are direct extensions of the original concepts of optimal control, relative weighting parameters are required amongst the cost and estimation error terms to make the criteria adjustable to the needs of a specific problem (see Bryson and Ho [26], or Athans [10] regarding the concepts of optimal control. See Athans [7], Kramer and Athans [73], Athans and Schweppe [12], Meier, *et al.* [92], Shoemaker and Lamont [117], Cooper and Nahi [27], Sauer and Melsa [107], Vande Linde and Lavi [125], Kushner [75], Sano and Terao [106], Dreyfus in Karreman [70], and particularly Aoki and Li [5] for examples of work in the area of optimal system design with measurement cost). The choice of such weighting parameters inevitably complicates the measurement system design problem. Particularly in applications in the environmental area, combining the minimization of costs associated with measuring a process with the minimization of a measure of the errors made in the estimation of the variables in that process does not seem to address the correct problem. In any practical implementation, legal limits would be placed upon estimation errors allowable in the pollutant estimates. On the other hand, the use of a combined performance criterion typically admits arbitrarily high estimation error levels at certain points in time, since the objective of the optimization is to minimize the time integral of the performance criterion, not its instantaneous value. Thus, the minimization of a performance criterion involving the time integral of a weighted combination of measurement cost and estimation error is not solving the right problem in the context of an environmental monitor.

Thus, the separation of the optimal monitoring problem into the problems of optimal design and management leads to a problem structure which conforms better to the requirements in actual applications than

do those which come from the application of principles of optimal control with combined, quadratic performance indices.

If, at all measurement times, the cost of making a measurement of a given quality is a constant, then the total cost of the required monitoring program over the time interval of interest is directly related to the number of times a measurement of a given quality has to be made, scaled by some cost weighting factor which is typically a function of the accuracy of the measurement instrument involved. Roughly speaking, then, the total cost of the whole monitoring program is an increasing function of the total number of individual samples which must be taken over the time interval of interest in order to maintain the value of the selected estimation error criterion within its bound over that entire time interval. With this assignment of measurement cost as a function of measurement instrument accuracy, then, the two optimal monitoring problems to be considered in this study are defined as follows:

> The Optimal Monitoring Problem of the First Kind — Find the optimal number and quality of measurement devices, their optimal locations in the medium and the optimal measurement times such that the total cost for the measurements required to maintain the estimation error in the state of system below a given bound over the time interval of interest is minimized. (2.7)

> The Optimal Monitoring Problem of the Second Kind — Find the optimal number and quality of measurement devices, their optimal locations in the medium and the optimal measurement times such that the total cost for the measurements required to maintain the maximum estimation error in the pollutant concentration anywhere in the medium below a given bound over the time interval of interest is minimized. (2.8)

Notice that in the above problem definitions, the choice of model complexity for use in the monitor — the order of the model and perhaps certain aspects of its structure — has been excluded. It is reintroduced later in Chapter 6 in a sensitivity analysis of monitor performance

as a function of the number of normal mode states retained in the series solution approximation for the dynamic equations involved.

In what follows, the problem stated in (2.7) or (2.8) are equivalently referred to as the optimal monitoring problems with bound on error in the state or output estimate, respectively.

The next chapter considers normal mode models for pollutant transport which result in sets of first-order, ordinary differential equations of the initial value type; these are commonly known in system theory as continuous-time state equations (see Desoer [32]).

In Chapter 4, these continuous-time state equations are discretized in time (see Freeman [41]) for computational implementation and for use in the Kalman Filter in the optimal estimation problem. In Chapter 5, attention is finally returned to consideration of the monitoring problems stated above.

CHAPTER 3. NORMAL MODE MODELS FOR DIFFUSIVE SYSTEMS

The transport and dispersal of a particular pollutant in some region P can be described by the following partial differential equation:

$$\frac{\partial F}{\partial t} = -\vec{\underset{\sim}{U}} \cdot \vec{\underset{\sim}{\nabla}} F + \frac{1}{\rho} \vec{\underset{\sim}{\nabla}} \cdot \rho K \vec{\underset{\sim}{\nabla}} F - \alpha F + f + g \qquad (3.1)$$

where

F = mixing ratio of pollutant (grams of pollutant per kilogram of medium);

$\vec{\underset{\sim}{\nabla}}$ = gradient operator;

$\vec{\underset{\sim}{U}}$ = local velocity of medium;

ρ = mass density;

K = diffusivity coefficient;

α = scavenging rate coefficient;

f = stochastic pollutant source term (grams pollutant per unit time per kilogram of medium);

and finally

g = deterministic pollutant source term (same units as f).

The terms of the right-hand side of (3.1) represent, respectively, (1) forced convection (or advection), (2) Fickian diffusion, (3) environmental degradation (or scavenging) of pollutant from the region, (4) stochastic and (5) deterministic pollutant production within the region.

For some environmental media, particularly the atmosphere, the properties ρ and K vary in space and time. In some cases, (3.1) will not be an accurate description where K may also vary with direction of diffusion and/or the scavenging term may require a far more complicated description. The above equation describes the transport of only a single pollutant species, F; if more than one pollutant is being considered, an equation

like (3.1) is required for each one where more terms may be necessary to describe chemical reactions among the various pollutants if they exist. Another case where (3.1) may be an incomplete description is with a meteorologically or hydrologically active pollutant, one which can change the energy balance of the medium; an example is a pollutant whose presence effects optical properties within the region. For this latter case, the full energy and momentum equations of fluid mechanics must be augmented to (3.1) to complete the mathematical description of pollutant dispersal [35,36]. Thus, modeling pollutant transport in general is seen to involve a great deal of analytical difficulty.

While approaches to the solution of (3.1) typically evolve from the use of finite difference methods [80,81,99], the extensions of modal analysis techniques proposed by Young [131] to pollutant transport problems will be used in this study. The powerful results which come from the application of normal mode analysis are felt to extend directly to finite difference models as will be suggested at the end of this report; thus, use of normal mode models is not a real restriction.

In order to gain insight into the mathematical relationships involved in monitoring the dispersion of pollutants in time and space, consider a more tractable simplified version of (3.1), namely

$$\frac{\partial \xi}{\partial t} = K\nabla^2\xi - \alpha\xi + f + g \tag{3.2}$$

where

ξ = concentration of pollutant (grams of pollutant per cubic meter of medium).

The simplifications adopted in using (3.2) in place of (3.1) include the following: mass density ρ is assumed to be constant, which allows the use of concentration instead of mixing ratio as the dependent variable

when the fluid can be assumed incompressible; spatial variation of the diffusivity K is negligible and advection is dominated by diffusion as the principle mechanism of transport.

Since (3.2) is linear in ξ, and since the main emphasis of this study is upon the stochastic nature of its solution, the deterministic source term may be eliminated since its effects could be added later to the stochastic solution by the method of superposition. The result is

$$\frac{\partial \xi}{\partial t} = K\nabla^2\xi - \alpha\xi + f. \tag{3.3}$$

This equation forms the basis for this study. It is the stochastic diffusion equation including scavenging written in arbitrary coordinates (it should be noted that (3.3) equally well describes stochastic heat transfer in solids including radiation to the surroundings).

The above assumptions mean that applications of the results which follow to problems in atmospheric pollution are remote at best. However, (3.3) is sometimes used for long time scales in global atmospheric studies (see references cited in [131]). In such cases, ξ is interpreted as the pollutant concentration averaged over mixing times sufficiently long that local wind velocities can be viewed as small scale effects of large scale eddies. However, application of the results to be developed around (3.3) are thought to be possible in groundwater systems or those surface water systems for which local velocities are small.

It should be noted that spatial variation in the density and diffusivity can be reintroduced into the problem to extend the results of this work to inhomogeneous anisotropic regions. This can be done by dividing the region P into component subregions in each of which the assumption of constant ρ and K is a reasonable approximation. Young [131]

has shown that by coupling such component submodels together, low order models of relatively high accuracy are able to be formed.

For now ignore the inclusion of pollutant scavenging in the transport equation. It will be introduced later as it effects the results for the optimal monitoring problem for diffusive transport alone in Chapter 5. Thus, with this final simplification, the stochastic partial differential equation governing Fickian diffusion results:

$$\frac{\partial \xi}{\partial t} = K\nabla^2\xi + f. \tag{3.4}$$

Various methods exist for solving (3.4) but owing to its simplicity and useful areas of application, the method of separation of variables will be used to convert (3.4) into an infinite expansion of ordinary differential equations in time whose solutions multiply related eigenfunctions in space. Study has been made of the number of terms to retain in the expansion for adequate accuracy [131]. Determination of this number will not be of concern here though its importance will be demonstrated by example in Chapter 6.

Development of a finite set of continuous-time state equations of the form

$$\dot{\underline{x}} = \underline{\underline{A}}\underline{x} + \underline{w} \tag{3.5}$$

$$\underline{y} = \underline{\underline{C}}\underline{x} + \underline{v} \tag{3.6}$$

from the application of the method of separation of variables to (3.4) is followed by developments for problems with media of various dimensions in the remainder of this chapter. More rigorous theory regarding the separation of variables technique is summarized and referenced in [131].

3.1 Separation of Variables for the Diffusion Equation

Here the solution of the inhomogeneous stochastic diffusion equation (3.4) in arbitrary coordinates is expressed as a finite set of normal mode state equations of the form (3.5) with the use of the method of variation of parameters (see Berg and McGregor [18], p. 152).

Begin by considering the homogeneous counterpart to (3.4), namely

$$\frac{\partial \xi}{\partial t} = K\nabla^2 \xi. \tag{3.7}$$

Assume a solution for ξ of the form

$$\xi(P,t) = x(t)e(P) \tag{3.8}$$

where P is some point in the medium $\mathcal{P}$. Substitute this into (3.7) to obtain

$$\dot{x}(t)e(P) = Kx(t)\nabla^2 e(P) \tag{3.9}$$

or

$$\frac{\dot{x}(t)}{x(t)} = \frac{K\nabla^2 e(P)}{e(P)} . \tag{3.10}$$

The left-hand side is a function of t and the right-hand side is a function of P so that for arbitrary P and t, both must equal a constant, the so-calle separation constant or eigenvalue. Choose this constant to be $-\lambda$ so that the following separated equations result:

$$\dot{x}(t) + \lambda x(t) = 0, \tag{3.11}$$

$$\nabla^2 e(P) + \frac{\lambda}{K} e(P) = 0. \tag{3.12}$$

The equation in time, (3.11), is already seen to be in the form sought in (3.5). The spatial equation, (3.12), is the Helmholtz equation which, together with the boundary conditions for the medium, forms an eigenproblem over $\mathcal{P}$, the region of interest. The resultant eigenfunctions $e_n(P)$ can be used to form bases for solutions of (3.7); assume a solution of the form

$$\xi(P,t) = \sum_{n=1}^{\infty} x_n(t)e_n(P). \tag{3.13}$$

Substitute this into the inhomogeneous diffusion equation (3.4) to obtain

$$\sum_{n=1}^{\infty} \dot{x}_n(t)e_n(P) = K\sum_{n=1}^{\infty} x_n(t)\nabla^2 e_n(P) + f(P,t). \tag{3.14}$$

The eigenfunctions are distinguished by the property of orthogonality, which can be stated as

$$\int_P e_n(P)e_m(P)\,dp = \begin{cases} 0 & n \neq m \\ 1 & n = m \end{cases} \tag{3.15}$$

the integration occurring over the whole region P. Use this property in (3.14) together with (3.12) to obtain

$$\sum_{n=1}^{\infty} \dot{x}_n(t)\int_P e_n(P)e_m(P)\,dp = -K\sum_{n=1}^{\infty} x_n(t)\frac{\lambda_n}{K}\int_P e_n(P)e_m(P)\,dp + \int_P f(P,t)e_m(P)\,dp. \tag{3.16}$$

The orthogonality then reduces (3.16) to the following set of first order ordinary differential equations

$$\dot{x}_n(t) = -\lambda_n x_n(t) + \int_P f(P,t)e_n(P)\,dp. \tag{3.17}$$

The integral in (3.17) is the contribution to the nth mode due to the source term $f(P,t)$. If $f(P,t)$ can be expanded in a series of eigenfunctions it can be given by

$$f(P,t) = \sum_{n=1}^{\infty} f_n(t)e_n(P). \tag{3.18}$$

Multiply by $e_m(P)$, integrate over the region and apply orthogonality again to obtain

$$f_n(t) = \int_P f(P,t)e_n(P)\, dp, \tag{3.19}$$

where $f_n(t)$ is the modal input for the nth differential equation. Thus wit .19), (3.17) may be written in the compact form

$$\dot{x}_n(t) = -\lambda_n x_n(t) + f_n(t), \qquad n = 1,2,\ldots . \tag{3.20}$$

This infinite sequence of ordinary differential equations is known as the set of normal mode state equations and together with the mode shapes given by the eigenfunctions $e_n(P)$, they comprise the normal mode solution in (3.13) of the inhomogeneous diffusion equation (3.4).

The remainder of this chapter will concern forms for the eigenfunctions $e_n(P)$, the spatial side of the problem. This will involve solving for the eigenfunctions once the coordinate systems are specified and boundary conditions given. Thus, finding $e_n(P)$, the eigenvalues λ_n and solving for the source terms $f_n(P)$ will be considered next for a range of different problems. Solving for the time response $x_n(t)$ will be approached in Chapter 4.

3.2 One-Dimensional Diffusion

Here will be considered the problem of diffusion in a one-dimensional medium. Classically, this is the problem of heat conduction between two infinite parallel flat plates. The problem also embraces that of pollutant diffusion where diffusivity constants dominate in one coordinate

direction only. Consider, then, the system described schematically as follows:

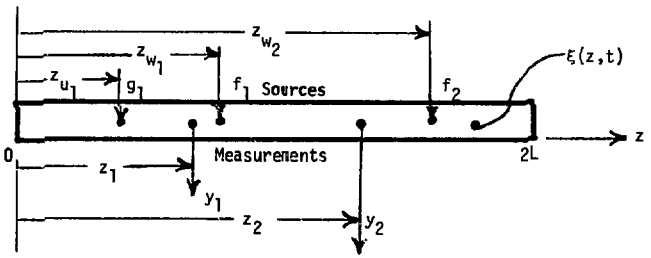


Figure 3.1.

3.2.1 No-Flow Boundary Conditions — For the system of length 2L described in Figure 3.1, the following specifies the related initial-boundary value problem:

$$\frac{\partial \xi(z,t)}{\partial t} = K \frac{\partial^2 \xi(z,t)}{\partial z^2} + f(z,t) + g(z,t); \tag{3.21}$$

$$\frac{\partial}{\partial z}\xi(0,t) \equiv 0, \qquad \frac{\partial}{\partial z}\xi(2L,t) \equiv 0; \tag{3.22}$$

$$\xi(z,0) \equiv \xi_0; \tag{3.23}$$

$$f_1(z,t) \equiv w_1(t)\delta\left(z - z_{w_1}\right), \tag{3.24}$$

$$E\left[w_1(t)\right] = 0, \tag{3.24A}$$

$$E\left[w_1(t)w_1(\tau)\right] = W_1\delta(t - \tau); \tag{3.24B}$$

$$f_2(z,t) \equiv w_2(t)\delta\left(z - z_{w_2}\right), \tag{3.25}$$

$$E\left[w_2(t)\right] = 0, \tag{3.25A}$$

$$E\left[w_2(t)w_2(\tau)\right] = W_2\ \delta(t - \tau); \tag{3.25B}$$

$$g_1(z,t) \equiv u_1(t)\ \delta\left(z - z_{u_1}\right). \tag{3.26}$$

Thus, the system represents diffusion in a one-dimensional medium of length 2L and diffusivity K with no influx or efflux of the diffusing substance at the ends. The initial condition throughout the medium is chosen as a constant, ξ_0. There are two stochastic point sources, f_1 at $z = z_{w_1}$ and f_2 at z_{w_2}, with zero means and constant covariances given by W_1 and W_2, respectively. One deterministic source of strength $u_1(t)$ acts at $z = z_{u_1}$.

Measurements $y_1(t)$ and $y_2(t)$ are taken at points z_1 and z_2. Expressions for these measurements in terms of the resulting system of normal mode state variables are sought.

As in (3.13), begin the analysis by assuming a solution of (3.21) of the form

$$\xi(z,t) = \sum_{n=1}^{\infty} x_n(t)\ \cos\left((n - 1)\ \frac{\pi}{2L}\ z\right). \tag{3.27}$$

Substitute this into (3.21) to obtain

$$\sum_{n=1}^{\infty} \dot{x}_n(t)\ \cos\left((n - 1)\ \frac{\pi}{2L}\ z\right)$$

$$= -K \sum_{n=1}^{\infty} x_n(t)(n - 1)^2\ \frac{\pi^2}{4L^2}\ \cos\left((n - 1)\ \frac{\pi}{2L}\ z\right)$$

$$+ f(z,t) + g(z,t). \tag{3.28}$$

Right-multiply by $\cos\left((m-1)\ \frac{\pi}{2L}\ z\right)$, integrate over the length of the medium and invoke the orthogonality of the eigenfunctions to obtain

$$2L\dot{x}_n(t) = -(n-1)^2 \frac{K\pi^2}{2L} x_n(t) + \int_{}^{2L} f(z,t) \cos\left((n-1)\frac{\pi}{2L} z\right) dz$$

$$+ \int_{z=0}^{2L} g(z,t) \cos\left((n-1)\frac{\pi}{2L} z\right) dz, \qquad n = 1; \tag{3.29}$$

$$L\dot{x}_n(t) = -(n-1)^2 \frac{K\pi^2}{2L} x_n(t) + \int_{z=0}^{2L} f(z,t) \cos\left((n-1)\frac{\pi}{2L} z\right) dz$$

$$+ \int_{z=0}^{2L} g(z,t) \cos\left((n-1)\frac{\pi}{2L} z\right) dz, \qquad n = 2,3,\ldots, \tag{3.30}$$

The above may be generalized into one infinite set of first-order ordinary differential equations in state-space form first by making the definitions:

	R_n	C_n
$n = 1$	$\frac{2L}{(n-1)^2 K\pi^2}$	$2L$
$n = 2,3,\ldots$	$\frac{2L}{(n-1)^2 K\pi^2}$	L

(3.31)

With these definitions, the complete normal mode solution for the one-dimensional stochastic diffusion equation, equation (3.21), may be written as the sequence

$$\dot{x}_n(t) = -\frac{1}{R_n C_n} x_n(t) + \frac{1}{C_n} \int_{z=0}^{2L} f(z,t) \cos\left((n-1)\frac{\pi}{2L} z\right) dz$$

$$+ \frac{1}{C_n} \int_{z=0}^{2L} g(z,t) \cos\left((n-1)\frac{\pi}{2L} z\right) dz, \qquad n = 1,2,\ldots . \tag{3.32}$$

Thus, the concentration $\xi(z,t)$ is found by solving the modal equations (3.32) and substituting into the assumed solution (3.27). To do this,

the solution must fit the initial condition so that

$$\xi_0 = \sum_{n=1}^{\infty} x_n(0) \cos\left((n - 1) \frac{\pi}{2L} z\right). \tag{3.33}$$

For this case, it is easily seen that

$$\begin{aligned} x_1(0) &\equiv \xi_0 \\ x_n(0) &\equiv 0, \qquad n = 2,3,\ldots . \end{aligned} \tag{3.34}$$

Point sources are the most straightforward types of inputs to represent in normal mode form (see Mac Robert [82], p. 124). The stochastic and deterministic sources are transformed as follows:

$$\begin{aligned} &\frac{1}{C_n} \int_{z=0}^{2L} f_1(z,t) \cos\left((n - 1) \frac{\pi}{2L} z\right) dz \\ &\quad = \frac{1}{C_n} \int_{z=0}^{2L} w_1(t)\delta\left(z - z_{w_1}\right) \cos\left((n - 1) \frac{\pi}{2L} z\right) dz \\ &\quad = \left[\frac{1}{C_n} \cos\left((n - 1) \frac{\pi}{2L} z_{w_1}\right)\right] w_1(t), \qquad n = 1,2,\ldots . \end{aligned} \tag{3.35A}$$

Similarly, for $f_2(z,t)$,

$$\begin{aligned} &\frac{1}{C_n} \int_{z=0}^{2L} f_2(z,t) \cos\left((n - 1) \frac{\pi}{2L} z\right) dz \\ &\quad = \left[\frac{1}{C_n} \cos\left((n - 1) \frac{\pi}{2L} z_{w_2}\right)\right] w_2(t), \qquad n = 1,2,\ldots . \end{aligned} \tag{3.35B}$$

The deterministic term is

$$\frac{1}{C_n}\int_{z=0}^{2L} g(z,t)\cos\left((n-1)\frac{\pi}{2L}z\right)dz$$

$$=\left[\frac{1}{C_n}\cos\left((n-1)\frac{\pi}{2L}z_{u_1}\right)\right]u_1(t), \qquad n=1,2,\ldots . \tag{3.36}$$

If the infinite series in (3.13) and (3.27) are truncated after term n, the retained modal equation may be written as follows:

$$\begin{bmatrix}\dot{x}_1\\ \dot{x}_2\\ \vdots\\ \dot{x}_n\end{bmatrix}=\begin{bmatrix}0 & & \bigcirc\\ -\frac{K\pi^2}{4L^2} & & \\ & \ddots & \\ \bigcirc & & -(n-1)^2\frac{K\pi^2}{4L^2}\end{bmatrix}\begin{bmatrix}x_1\\ x_2\\ \vdots\\ x_n\end{bmatrix}$$

$$+\begin{bmatrix}\frac{1}{2L} & \frac{1}{2L}\\ \frac{1}{L}\cos\left(\frac{\pi}{2L}z_{w_1}\right) & \frac{1}{L}\cos\left(\frac{\pi}{2L}z_{w_2}\right)\\ \vdots & \vdots\\ \frac{1}{L}\cos\left((n-1)\frac{\pi}{2L}z_{w_1}\right) & \frac{1}{L}\cos\left((n-1)\frac{\pi}{2L}z_{w_2}\right)\end{bmatrix}\begin{bmatrix}w_1\\ w_2\end{bmatrix}+\begin{bmatrix}\frac{1}{2L}\\ \frac{1}{L}\cos\left(\frac{\pi}{2L}z_{u_1}\right)\\ \vdots\\ \frac{1}{L}\cos\left((n-1)\frac{\pi}{2L}z_{u_1}\right)\end{bmatrix}u_1 . \tag{3.37}$$

with initial condition

$$\begin{bmatrix}x_1(0)\\ x_2(0)\\ \vdots\\ x_n(0)\end{bmatrix}=\begin{bmatrix}\xi_0\\ 0\\ \vdots\\ 0\end{bmatrix}. \tag{3.38}$$

The noise-corrupted measurements

$$\begin{bmatrix}y_1\\ y_2\end{bmatrix}=\begin{bmatrix}1 & \cos\left(\frac{\pi}{2L}z_1\right) & \cdots & \cos\left((n-1)\frac{\pi}{2L}z_1\right)\\ 1 & \cos\left(\frac{\pi}{2L}z_2\right) & \cdots & \cos\left((n-1)\frac{\pi}{2L}z_2\right)\end{bmatrix}\begin{bmatrix}x_1\\ x_2\\ \vdots\\ x_n\end{bmatrix}+\begin{bmatrix}v_1\\ v_2\end{bmatrix}. \tag{3.39}$$

In summary, the stochastic initial-boundary value problem (3.21) - (3.26) has been transformed through the method of separation of variables into a truncated sequence of first order ordinary differential equations (3.37) with initial conditions (3.38). Measurements made of the system are expressed as in (3.39). These equations comprise the state and output equations which may be written as

$$\dot{\underset{\sim}{x}} = \underset{\sim}{A}\underset{\sim}{x} + \underset{\sim}{D}\underset{\sim}{w} + \underset{\sim}{B}\underset{\sim}{u}, \tag{3.40}$$

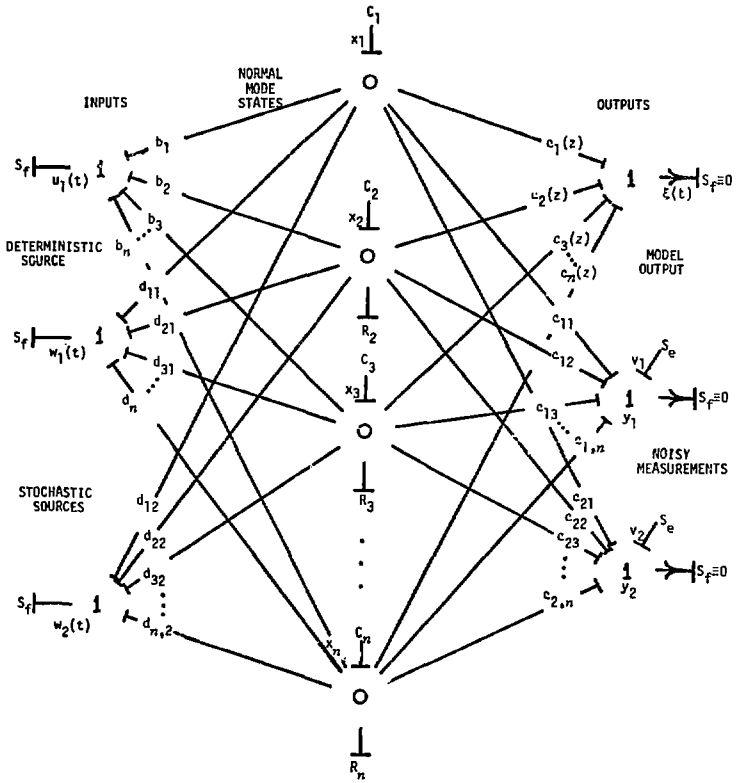
$$\underset{\sim}{y} = \underset{\sim}{C}\underset{\sim}{x} + \underset{\sim}{v}. \tag{3.6}$$

As in equation (3.4), most of the examples of interest here will exclude terms like $\underset{\sim}{B}\underset{\sim}{u}$ in (3.40).

Once the truncated sequence of normal mode state equations is determined, the resulting pollutant concentration at any point z in the medium for any time t may be found as follows:

$$\xi(z,t) = \sum_{n=1}^{n} x_n(t) \cos\left((n - 1)\frac{\pi}{2L} z\right). \tag{3.41}$$

Finally, insight into the structure of the finite normal mode model of the one-dimensional diffusion process may be gained by portraying relationships (3.37), (3.38), (3.39), and (3.41) in a bond graph [69]; see Figure 3.2. The table at the bottom of the figure defines the functional relationships involved in the coefficients b, c, and d; these are in actuality all modulated transformer elements.



	R_n	C_n	b_n	d_{nm}	c_{yn}	$c_n(z)$
$n = 1$	-	$2L$	$\frac{1}{2L}$	$\frac{1}{2L}$	1	1
$n = 2,3,\ldots,n$	$\frac{2L}{(n-1)^2\pi^2}$	L	$\frac{1}{L}\cos\left((n-1)\frac{\pi}{2L}z_{u_1}\right)$	$\frac{1}{L}\cos\left((n-1)\frac{\pi}{2L}z_{w_m}\right)$	$\cos\left((n-1)\frac{\pi}{2L}z_r\right)$	$\cos\left((n-1)\frac{\pi}{2L}z\right)$

Figure 3.2. Bond graph of normal mode state, measurement and output equations used in the monitoring problem.

3.2.2 Fixed Boundary Conditions — Consider the initial-boundary value problem

$$\frac{\partial \xi(z,t)}{\partial t} = K \frac{\partial^2 \xi(z,t)}{\partial z^2} + f(z,t); \tag{3.42}$$

$$\xi(0,t) = 0, \qquad \xi(2L,t) = 0; \tag{3.43}$$

$$\xi(z,0) = 0; \tag{3.44}$$

$$f(z,t) = w(t)\delta(z - z_w), \tag{3.45}$$

$$E[w(t)] = 0 \tag{3.46}$$

$$E[w(t)w(\tau)] = W\delta(t - \tau). \tag{3.47}$$

The essential difference from the problem in Section 3.2.1 is in the nature of the boundary conditions. The so-called "fixed" boundary conditions of (3.43) are referred to as the Dirichlet conditions by others (see Berg and Mc Gregor [18], Section 3.6). They represent the physically rare situation where the pollutant concentrations at the ends of the medium are fixed to some specified source levels as functions of time; here those levels are arbitrarily chosen to be zero. This difference manifests itself in the form for the eigenfunctions, $e_n(z)$, and eigenvalues, λ_n.

In this case, assume a solution of (3.42) of the form

$$\xi(z,t) = \sum_{n=1}^{\infty} x_n(t) \sin\left(n \frac{\pi}{2L} z\right). \tag{3.48}$$

Substitute (3.48) into (3.42), right multiply by $\sin\left(m \frac{\pi}{2L} z\right)$, integrate over the length of the medium and invoke orthogonality to obtain

$$L\dot{x}_n(t) = -n^2 \frac{K\pi^2}{4L} x_n(t) + \int_{z=0}^{2L} f(z,t) \sin\left(\frac{n\pi}{2L} z\right) dz. \tag{3.49}$$

As before, generalized modal resistances and capacitances may be defined:

$n = 1,2,\ldots$	R_n	C_n
	$\frac{4L}{n^2K\pi^2}$	L

(3.50)

Thus, the general modal state equation is

$$\dot{x}_n(t) = -\frac{1}{R_nC_n}x_n(t) + \frac{1}{C_n}\int_{z=0}^{2L} f(z,t)\sin\left(n\frac{\pi}{2L}z\right)dz. \quad (3.51)$$

The general solution (3.48) must satisfy the initial condition, or

$$\xi(z,0) = 0 = \sum_{n=1}^{\infty} x_n(0)\sin\left(n\frac{\pi}{2L}z\right), \quad (3.52)$$

from which

$$x_n(0) = 0, \qquad n = 1,2,\ldots . \quad (3.53)$$

The stochastic forcing term is treated in a manner similar to (3.35A) for the case with no-flow boundary conditions.

If the infinite series in (3.48) is truncated after term n the finite set of normal mode state equations results as follows:

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \vdots \\ \dot{x}_n \end{bmatrix} = \begin{bmatrix} -\frac{K\pi^2}{4L^2} & & & \bigcirc \\ & -4\frac{K\pi^2}{4L^2} & & \\ & & \ddots & \\ \bigcirc & & & (n)^2\frac{K\pi^2}{4L^2} \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} + \begin{bmatrix} \frac{1}{C}\sin\left(\frac{\pi}{2L}z_w\right) \\ \frac{1}{C}\sin\left(2\frac{\pi}{2L}z_w\right) \\ \vdots \\ \frac{1}{C}\sin\left(n\frac{\pi}{2L}z_w\right) \end{bmatrix} w(t) \quad (3.54)$$

Note that the major difference in the dynamics between systems with no-flow at the boundaries (as in Section 3.2.1) and systems with fixed boundary concentrations (as in this section) is in the first element of

the matrix $\underline{A}$. In the former, it is zero; in the latter, it is less than zero. This implies that the initial condition of the first mode of the problem with no flow at the boundaries will remain unchanged in time whereas that of the fixed boundary concentration problem will vanish for large time. This difference is central to the considerations of Chapter 5.

3.3 Two-Dimensional Diffusion

Consider the diffusion of a pollutant in a thin, flat, three-dimensional volume. For simplicity, consider the region to be of rectangular shape with sides of lengths $2L_1$, $2L_2$, and $2L_3$ in the ζ_1, ζ_2, and ζ_3 coordinate directions, as shown in Figure 3.3.

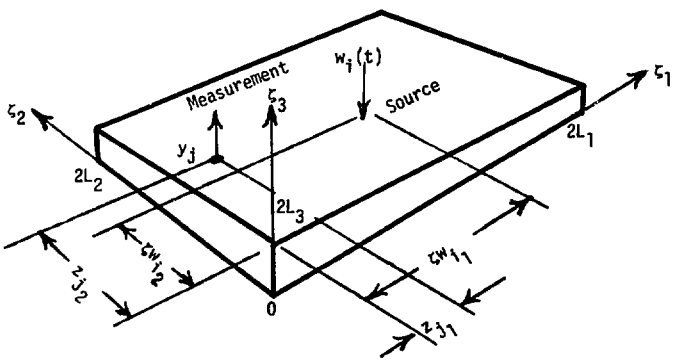


Figure 3.3.

If the vertical height $2L_3$ is small in comparison to the horizontal dimensions $2L_2$ and $2L_3$, the gradient of the pollutant concentration in the ζ_3 direction can be neglected so that the average concentration in the vertical direction can be assumed for the concentration throughout the vertical dimension for any horizontal location.

Two dimensional diffusion applies to such a simplified model. Consider the case of diffusion in a homogeneous medium with no-flow boundary conditions and with r stochastic point sources at various locations in the medium. The initial-boundary value problem in two dimensions may be written for this model as follows:

$$\frac{\partial \xi(\underset{\sim}{\zeta},t)}{\partial t} = K\left(\frac{\partial^2 \xi(\underset{\sim}{\zeta},t)}{\partial \zeta_1^2} + \frac{\partial^2 \xi(\underset{\sim}{\zeta},t)}{\partial \zeta_1^2}\right) + f(\underset{\sim}{\zeta},t); \tag{3.55}$$

$$\frac{\partial \xi(\underset{\sim}{\zeta},t)}{\partial \zeta_1} = 0, \qquad \zeta_1 = 0, \quad \zeta_1 = 2L_1,$$

$$\frac{\partial \xi(\underset{\sim}{\zeta},t)}{\partial \zeta_2} = 0, \qquad \zeta_2 = 0, \quad \zeta_2 = 2L_2; \tag{3.56}$$

$$\xi(\underset{\sim}{\zeta},0) = \xi_0; \tag{3.57}$$

$$f_i(\underset{\sim}{\zeta},t) = w_i(t)\delta\left(\zeta_1 - \zeta_{w_{i_1}}\right)\delta\left(\zeta_2 - \zeta_{w_{i_2}}\right),$$

$$E[w_i(t)] = 0,$$

$$E[w_i(t)w_i(\tau)] = W_i\delta(t - \tau), \qquad i = 1,2,\ldots,r. \tag{3.58}$$

The no-flow boundary conditions (3.56) correspond to the case which has interesting practical applications where many such models may be coupled together to span a larger, possibly inhomogeneous, region. The initial pollutant concentration throughout the medium is chosen to be a constant in the initial condition (3.57) for simplicity. r individual stochastic point sources, each located at $\underset{\sim}{\zeta}_{w_i} \equiv \left[\zeta_{w_{i_1}}, \zeta_{w_{i_2}}\right]^T$, are described by the relationships in (3.58).

The separation of variables of this two-dimensional initial-boundary value problem proceeds much like the one-dimensional case. However, in this case, owing to the inclusion of two spatial dimensions, the

eigenfunctions in the general case (3.13) will be products of independent functions of the two space variables as follows:

$$e_{nm}(\underset{\sim}{\zeta}) \equiv e_n(\zeta_1)e_m(\zeta_2) = \cos\left((n-1)\frac{\pi}{2L_1}\zeta_1\right)\cos\left((m-1)\frac{\pi}{2L_2}\zeta_2\right). \quad (3.59)$$

Thus, assume a solution for (3.55) of the form

$$\xi(\underset{\sim}{\zeta},t) = \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} x_{nm}(t)e_{nm}(\underset{\sim}{\zeta})$$

$$= \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} x_{nm}(t)\cos\left((n-1)\frac{\pi}{2L_1}\zeta_1\right)\cos\left((m-1)\frac{\pi}{2L_2}\zeta_2\right). \quad (3.60)$$

This is a direct extension of the one-dimensional form in (3.27).

Applying the same techniques used in the one-dimensional problem leads to the following resultant normal mode problem formulation for the two-dimensional case (for details, see Young [131], p. 76, Duff and Naylor [34], p. 148, Mac Robert [81], § 13 and particularly Berg and Mc Gregor [18], Chapter 10).

Define the generalized modal resistances and capacitances R_ν and C_ν as in (3.31) where ν is either n or m as in (3.59), and μ is either 1 or 2 to correspond with coordinate ζ_1 or ζ_2, as follows:

	R_ν	C_ν
$\nu = 1$	$\frac{2L_\mu}{(\nu-1)^2L\pi^2}$	$2L_\mu$
$\nu = 2,3,\ldots$	$\frac{2L_\mu}{(\nu-1)^2K\pi^2}$	L_μ

(3.61)

As in the one-dimensional case, substitute the assumed solution $\xi(\underset{\sim}{\zeta},t)$ given in (3.60) into the differential equation (3.55), right-multiply by eigenfunction $e_{qr}(\underset{\sim}{\zeta})$, integrate over the medium and use orthogonality.

Transform the initial condition (3.57) in a manner similar to (3.33) and (3.34) and the set of r stochastic point sources as was done in (3.35A). Truncate the double-infinite series solution in (3.60) to include n terms in each coordinate direction in order to obtain the following finite set of n^2 normal mode state equations:

$$\begin{bmatrix} \dot{x}_{11} \\ \dot{x}_{21} \\ \vdots \\ \dot{x}_{n,1} \\ \dot{x}_{1,2} \\ \vdots \\ \dot{x}_{nn} \end{bmatrix} = \begin{bmatrix} 0 & & & & & & \bigcirc \\ -\left(\frac{1}{R_2C_2}+\frac{1}{R_1C_1}\right) & & & & & & \\ & \ddots & & & & & \\ & & -\left(\frac{1}{R_nC_n}+\frac{1}{R_1C_1}\right) & & & & \\ & & & -\left(\frac{1}{R_1C_1}+\frac{1}{R_2C_2}\right) & & & \\ & & & & \ddots & & \\ \bigcirc & & & & & -\left(\frac{1}{R_nC_n}+\frac{1}{R_nC_n}\right) & \end{bmatrix} \begin{bmatrix} x_{11} \\ x_{21} \\ \vdots \\ x_{n,1} \\ x_{1,2} \\ \vdots \\ x_{nn} \end{bmatrix}$$

$$+ \begin{bmatrix} \frac{1}{C_1C_1}(1)(1) & \frac{1}{C_1C_1}(1)\cos\left(\frac{\pi}{2L_2}\zeta_{w_{2_2}}\right)\cdots \\ \frac{1}{C_2C_2}\cos\left(\frac{\pi}{2L_1}\zeta_{w_{1_1}}\right)(1) & \frac{1}{C_2C_1}\cos\left(\frac{\pi}{2L_1}\zeta_{w_{2_1}}\right)\cos\left(\frac{\pi}{2L_2}\zeta_{w_{2_2}}\right)\cdots \\ \vdots & \vdots \\ & \frac{1}{C_nC_n}\cos\left((n-1)\frac{\pi}{2L_1}\zeta_{w_{r_1}}\right)\cos\left((n-1)\frac{\pi}{2L_2}\zeta_{w_{r_2}}\right) \end{bmatrix} \begin{bmatrix} w_1(t) \\ w_2(t) \\ \vdots \\ w_r(t) \end{bmatrix} \tag{3.62}$$

with initial condition given by

$$\begin{bmatrix} x_{11}(0) \\ x_{21}(0) \\ \vdots \\ x_{n_1 1}(0) \\ x_{12}(0) \\ \vdots \\ x_{nn}(0) \end{bmatrix} \equiv \begin{bmatrix} \xi_0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \tag{3.63}$$

For m noise-corrupted measurements

$$\underset{\sim}{y} = \underset{\sim}{C}\underset{\sim}{x} + \underset{\sim}{v}; \tag{3.6}$$

as in the one-dimensional case, the measurement equation is written as follows:

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix} = \begin{bmatrix} (1)(1) & \cos\left(\frac{\pi}{2L_1} z_{1_1}\right)(1) & \cdots \\ (1)(1) & \cos\left(\frac{\pi}{2L_1} z_{2_1}\right)\cos\left(\frac{\pi}{2L_2} z_{2_2}\right) & \cdots \\ \vdots & \vdots & \\ (1)(1) & \cdots & \cos\left((n-1)\frac{\pi}{2L_1} z_{m_1}\right)\cos\left((n-1)\frac{\pi}{2L_2} z_{m_2}\right) \end{bmatrix} \begin{bmatrix} x_{11}(t) \\ x_{21}(t) \\ \vdots \\ x_{nn}(t) \end{bmatrix} + \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_m \end{bmatrix} \tag{3.64}$$

In the state equation (3.62), the position of the i<u>th</u> point source is written as

$$\underset{\sim}{\zeta}_{w_i} \equiv \begin{bmatrix} \zeta_{w_{i_1}} \\ \zeta_{w_{i_2}} \end{bmatrix} \tag{3.65}$$

where the components in each coordinate direction ζ_1 and ζ_2 are as in

Figure 3.3. Similarly for the jth measurement position in the measurement equation (3.64).

$$\underline{z}_j \equiv \begin{bmatrix} z_{j_1} \\ z_{j_2} \end{bmatrix}, \tag{3.66}$$

also as shown in Figure 3.3 (do not confuse the subscript j with time indices used in later chapters; here, locally, $\underline{z}_j$ means the vector of the coordinates of the jth measurement position).

The result is that the two-dimensional diffusion problem results in sets of normal-mode state and measurement equations which are directly related to those in the one-dimensional problem. The only differences are that here *sums* of the eigenvalues occur in the diagonal $\underline{A}$ matrix and *products* of the eigenfunctions occur in the $\underline{C}$ and $\underline{D}$ matrices. The order of the system, i.e., the number of states retained, goes as the product of the number of modes retained in each coordinate direction. Thus, for the same number of modes, n, for each coordinate, to obtain accuracy in the solution comparable to that for n modes in the one-dimensional problem, a total of $(n)^2$ modes must be included in the two-dimensional model. Dimensionality, thus, grows as the number of modes in one dimension to a power equal to the number of space coordinates describing the domain of the medium in the problem.

3.4 Three-Dimensional Diffusion

The results for the two-dimensional case can be extended directly to three-dimensional regions in applicable coordinate systems (see references listed in Section 3.3 for conditions under which this extension is possible). In this case, solutions may be assumed to be products of

eigenfunctions in the three spatial coordinates and may be written

$$\xi(\underset{\sim}{\zeta},t) = \sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\sum_{r=1}^{\infty} x_{nmr}(t)\, e_n(\zeta_1)e_m(\zeta_2)e_r(\zeta_3). \qquad (3.67)$$

The details of the development are identical to those in the two-dimensional case and lead to the same forms for the $\underset{\sim}{A}$, $\underset{\sim}{D}$, and $\underset{\sim}{C}$ matrices in (3.62) and (3.64) except that the diagonal elements of $\underset{\sim}{A}$ are sums of eigenvalues for eigenfunctions in three, not two, coordinate directions and the elements of $\underset{\sim}{D}$ and $\underset{\sim}{C}$ are triple products of the one-dimensional eigenfunctions. Dimensionality of the resultant system of state equations goes as $(n)^3$.

Three-dimensional examples are included in the discussion of monitoring systems in Chapter 5 where the development is carried further.

It should be pointed out that the method of separation of variables used in normal mode analysis applies in other coordiante systems as well (e.g., cylindrical and spherical). See any of the references cited in Section 3.3 for their development.

CHAPTER 4. MODEL DISCRETIZATION AND APPLIED OPTIMAL ESTIMATION

The purpose of this chapter is two-fold. First, the continuous-time normal mode state equation models of Chapter 3 are transformed into discrete-time recurrence relationships for use in the Kalman Filter. The statement of these discretization methods is separated from the continuous-time model development of the previous chapter since they stand alone and can be applied to a variety of modeling techniques which result in systems of first-order ordinary differential equations. In addition to the normal mode modeling techniques developed above, they would, for example, apply equally well to uncoupled differential-difference models resulting from applying modal analysis [79] to finite-difference models [47] or to models resulting from using collocation methods [94]. Thus, the discretization methods outlined here are general and form a logical connection between the more familiar theory of continuous-time dynamic processes commonly associated with distributed system modeling and the theory of discrete-time dynamic systems where the majority of applications have been limited to the fields of control system and aerospace system analysis and synthesis.

Second, the optimal estimation problem is defined and its solution with the Kalman Filter is stated. While details of its development are referenced in the literature, a concise summary of an algorithm combining the simulation of the response of the model of a physical process with all necessary calculations for the optimal estimation is included at the end of this chapter.

4.1 Discretization of the System Model

4.1.1 The System Model Equations — The systems under consideration are typically modeled with sets of continuous-time, first-order ordinary differential equations of the form

$$\dot{\underset{\sim}{x}} = \underset{\sim}{A}\underset{\sim}{x} + \underset{\sim}{B}\underset{\sim}{u} + \underset{\sim}{D}\underset{\sim}{w} \tag{4.1}$$

$$\underset{\sim}{y} = \underset{\sim}{C}\underset{\sim}{x} + \underset{\sim}{v} \tag{4.2}$$

where the *statistics* of the initial state $\underset{\sim}{x}(0)$, disturbance $\underset{\sim}{w}(t)$ and measurement error $\underset{\sim}{y}(t)$ are given by

$$\begin{aligned}
&E[\underset{\sim}{x}(0)] = \underset{\sim}{m}_0, \\
&E[\underset{\sim}{x}(0)\underset{\sim}{x}(0)^T] = \underset{\sim}{M}_0, \\
&E[\underset{\sim}{w}(t)] = \underset{\sim}{0}, \\
&E[\underset{\sim}{w}(t)\underset{\sim}{w}(\tau)^T] = \underset{\sim}{W}(t)\delta(t-\tau), \\
&E[\underset{\sim}{v}(t)] = \underset{\sim}{0}, \\
&E[\underset{\sim}{v}(t)\underset{\sim}{v}(\tau)^T] = \underset{\sim}{V}(t)\delta(t-\tau), \\
&E[\underset{\sim}{x}(0)\underset{\sim}{w}(t)^T] = \underset{\sim}{0}, \\
&E[\underset{\sim}{x}(0)\underset{\sim}{v}(t)^T] = \underset{\sim}{0}, \\
&E[\underset{\sim}{w}(t)\underset{\sim}{v}(\tau)] = \underset{\sim}{0}.
\end{aligned} \tag{4.3}$$

The discrete-time counterpart of the above is

$$\underset{\sim}{x}_{K+1} = \underset{\sim}{\Phi}(t_{K+1},t_K)\underset{\sim}{x}_K + \tilde{\underset{\sim}{u}}_{K+1} + \tilde{\underset{\sim}{w}}_{K+1} \tag{4.4}$$

$$\underset{\sim}{y}_{K+1} = \underset{\sim}{C}_{K+1}\underset{\sim}{x}_{K+1} + \underset{\sim}{v}_{K+1}, \tag{4.5}$$

where the driving functions are defined by

$$\tilde{\underline{u}}_{K+1} \equiv \int_{t_K}^{t_{K+1}} \underline{\Phi}(t_{K+1},t)\underline{B}(t)\underline{u}(t)\,dt \tag{4.6}$$

$$\tilde{\underline{w}}_{K+1} \equiv \int_{t_K}^{t_{K+1}} \underline{\Phi}(t_{K+1},t)\underline{D}(t)\underline{w}(t)\,dt. \tag{4.7}$$

These two terms are convolutions of the deterministic and stochastic inputs and $\underline{\Phi}(.,.)$, the state transition matrix defined by the matrix differential equation

$$\dot{\underline{\Phi}} = \underline{A}\underline{\Phi}, \qquad \underline{\Phi}(t,t) = \underline{I}. \tag{4.8}$$

In the above, the system matrices $\underline{A}$, $\underline{B}$, $\underline{C}$, and $\underline{D}$ may be functions of time. For the time-invariant case, however, certain simplifying observations and approximations may be made. Let the time step be fixed, i.e., $T \equiv (t_{K+1} - t_K)$ and obtain (see Appendix A)

$$\underline{\Phi}_{K+1}^{K} \equiv \underline{\Phi}(t_{K+1},t_K) = e^{\underline{A}T} = \underline{I} + \underline{A}T + \frac{(\underline{A}T)^2}{2!} + \frac{(\underline{A}T)^3}{3!} + \ldots, \tag{4.9}$$

$$\underline{\Psi}_{K+1}^{K} = (e^{\underline{A}T} - \underline{I})\underline{A}^{-1}\underline{B}$$

$$= T\left(\underline{I} + \frac{1}{2!}(\underline{A}T) + \frac{1}{3!}(\underline{A}T)^2 + \ldots\right)\underline{B}, \tag{4.10}$$

$$\underline{\Gamma}_{K+1}^{K} = (e^{\underline{A}T} - \underline{I})\underline{A}^{-1}\underline{D}$$

$$= T\left(\underline{I} + \frac{1}{2!}(\underline{A}T) + \frac{1}{3!}(\underline{A}T)^2 + \ldots\right)\underline{D}. \tag{4.11}$$

With these definitions, it is possible to discretize the problem which results in a form necessary for the Kalman Filter. The discrete form of the state equation becomes

$$\underline{x}_{K+1} = \underline{\Phi}_{K+1}^{K}\underline{x}_K + \underline{\Psi}_{K+1}^{K}\underline{u}_K + \underline{\Gamma}_{K+1}^{K}\underline{w}_K. \tag{4.12}$$

Here it is assumed that the input terms $\underset{\sim}{u}_K$ and $\underset{\sim}{w}_K$ are sampled at time t_K and held constant over the interval $t_K \leq t < t_{K+1}$, that is,

$$\left.\begin{aligned} \underset{\sim}{u}(t) &= \underset{\sim}{u}(t_K) \\ \underset{\sim}{w}(t) &= \underset{\sim}{w}(t_K) \end{aligned}\right\} \quad t_K \leq t < t_{K+1}. \tag{4.13}$$

This assumption reduces the calculation of the convolutions for $\tilde{\underset{\sim}{u}}_{K+1}$ and $\tilde{\underset{\sim}{w}}_{K+1}$ in (4.4) given by (4.6) and (4.7) to the far simpler matrix-vector multiplications in (4.12) above. This is possible since the matrix series for $\underset{\sim}{\Psi}^K_{K+1}$ and $\underset{\sim}{\Gamma}^K_{K+1}$ in (4.10) and (4.11) are analytically exact expressions for the convolutions when the variables are sampled and held as in (4.13).

The matrix series in (4.9) - (4.11) are clearly impossible to evaluate exactly. The truncation of those series to a practical balance between accuracy and computational load has been suggested by H. M. Paynter (see Brewer [22], Ch. 8). The number of terms k retained in the series is found as a function of the maximum size of the elements of the matrix $[\underset{\sim}{A}T]$. A bound on the size of the remainder in the series is used to determine where the series should be truncated. Standard integration techniques (e.g., Runge-Kutta or linear multistep methods) are not used here under the assumption that if the time stepsize $T \equiv (t_{K+1} - t_K)$ is sufficiently small, smaller than the smallest characteristic times in the system response, then the accuracy of the truncated series approximation will be sufficient for the purpose of this study.

4.1.2 The System Disturbance Statistics — It can be shown (Jazwinski [65], p. 100) that the convolution $\tilde{\underline{w}}_{K+1}$ of the stochastic variable $\underline{w}(t)$ in (4.7) is itself a zero-mean, white Gaussian sequence with covariance matrix given by

$$\underline{\Omega}_{K+1} \equiv E\left[\tilde{\underline{w}}_{K+1}\tilde{\underline{w}}_{K+1}^T\right] = \int_{t_K}^{t_{K+1}} \underline{\Phi}(t_{K+1},t)\underline{G}(t)\underline{W}(t)\underline{G}(t)^T\underline{\Phi}(t_{K+1},t)^T\,dt. \tag{4.14}$$

This term represents the increase in uncertainty in the estimate of the system state over the time interval $T \equiv (t_{K+1} - t_K)$ due to the stochastic disturbance term $\underline{w}(t)$ as in (4.1). This term is used in the error covariance equations in the Kalman Filter in the next section.

$\underline{W}(t)$ is a deterministic quantity so the integral in (4.14) does not involve a stochastic integrand. However, its numerical integration in general is still far from trivial. For this reason a recursive method for the evaluation of $\underline{\Omega}_{K+1}$ will be used, a method which closely follows the truncated series approximations for $\underline{\Phi}_{K+1}^K$, $\underline{\Psi}_{K+1}^K$, and $\underline{\Gamma}_{K+1}^K$ developed in Appendix A.

The development of the algorithm to compute $\underline{\Omega}_{K+1}$ is detailed in Appendix B. The method involves differentiating $\underline{\Omega}_{K+1}$ in (4.14) with respect to time, resulting in a matrix Riccati equation. Hamilton's equations are then found for the Riccati equation, which are then solved as a state transition equation. Partitions of its state transition matrix are shown to comprise the resultant expression for $\underline{\Omega}$. An iterative numerical technique (see D'Appolito [29]) is used in the actual implementation.

Suffice it to say here that a method is used to find state transition matrices $\underset{\sim}{\Phi}_{21}$ and $\underset{\sim}{\Phi}_{22}$ (see Appendix B) such that

$$\underset{\sim}{\Omega}_{K+1} = \underset{\sim}{\Phi}_{21}(T)\underset{\sim}{\Phi}_{22}(T)^T. \tag{4.15}$$

4.2 Optimal Estimation — The Kalman Filter

4.2.1 Optimal Estimation — State estimation in dynamic systems is covered widely in the literature. Various developments of the Kalman Filter for optimal estimation can be found in Kalman [66], Kalman and Bucy [69], Sorensen in Leondes [78], Sage [105], Bryson and Ho [26], Meditch [85], Jazwinski [65], and in an extensive Bibliography in IEEE [62].

The reader is referred to any of the above for analytical derivations of the Kalman Filter equations. The emphasis here is upon their implementation, taking advantage of properties peculiar to the models being used in this study.

The optimal estimation problem and its solution in the Kalman Filter are now described. Given is the discrete-time dynamical system described by the following difference equations:

$$\underset{\sim}{x}_{K+1} = \underset{\sim}{\Phi}^K_{K+1}\underset{\sim}{x}_K + \underset{\sim}{\Psi}^K_{K+1}\underset{\sim}{u}_K + \underset{\sim}{\Gamma}^K_{K+1}\underset{\sim}{w}_K \tag{4.16}$$

$$\underset{\sim}{y}_{K+1} = \underset{\sim}{C}_{K+1}\underset{\sim}{x}_{K+1} + \underset{\sim}{v}_{K+1}. \tag{4.17}$$

Here, $\underset{\sim}{x}_K$ is an n-vector, $\underset{\sim}{u}_K$ an p-vector, $\underset{\sim}{w}_K$ an r-vector, and $\underset{\sim}{y}_K$ and $\underset{\sim}{v}_K$ m-vectors. The vectors $\underset{\sim}{x}$, $\underset{\sim}{w}$, and $\underset{\sim}{v}$ are white, normally distributed random vectors with the following statistics:

$$
\begin{aligned}
&E[\underset{\sim}{x}_0] \equiv \underset{\sim}{m}_0, && E\left[\underset{\sim}{x}_0\ \underset{\sim}{x}_0^T\right] \equiv \underset{\sim}{M}_0 \\
&E[\underset{\sim}{w}_K] = \underset{\sim}{0}, && E\left[\underset{\sim}{w}_K\ \underset{\sim}{w}_j^T\right] = \underset{\sim}{W}_K\delta_{Kj} \\
&E[\underset{\sim}{v}_K] = \underset{\sim}{0}, && E\left[\underset{\sim}{v}_K\ \underset{\sim}{v}_j^T\right] = \underset{\sim}{V}_K\delta_{Kj} \\
&E\left[\underset{\sim}{x}_0\ \underset{\sim}{w}_K^T\right] = \underset{\sim}{0}, && E\left[\underset{\sim}{x}_0\ \underset{\sim}{v}_K^T\right] = \underset{\sim}{0}, \\
&E\left[\underset{\sim}{w}_K\ \underset{\sim}{v}_j^T\right] = \underset{\sim}{0}.
\end{aligned}
\tag{4.18}
$$

A notational convenience will be that for a normally distributed random vector $\underset{\sim}{\xi}$ with mean value $\underset{\sim}{\mu}$ and covariance $\underset{\sim}{\Sigma}$, $\underset{\sim}{\xi}$ is described as follows:

$$\underset{\sim}{\xi} \sim N(\underset{\sim}{\mu},\underset{\sim}{\Sigma}) \tag{4.19}$$

The recursive linear estimation problem for the system above is to determine an estimate $\hat{\underset{\sim}{x}}_K^K$ of the state $\underset{\sim}{x}$ at t_K that is a linear combination of an estimate at t_{K-1} and the measurement $\underset{\sim}{y}_K$ which minimizes the expected value of the sum of the squares of the errors in the estimate, that is, that estimate which minimizes

$$E\left[\left(\hat{\underset{\sim}{x}}_K^K - \underset{\sim}{x}_K\right)^T \left(\hat{\underset{\sim}{x}}_K^K - \underset{\sim}{x}_K\right)\right]. \tag{4.20}$$

It has been shown (see Kalman [66]) that the following comprises a filter which generates the "best" estimate in the mean-square sense of (4.20), of the state of the stochastic system (4.16) - (4.18).

The predicted error covariance matrix $\underset{\sim}{P}_{K+1}^K$ is defined by

$$\underset{\sim}{P}_{K+1}^K \equiv E\left[\left(\hat{\underset{\sim}{x}}_{K+1}^K - \underset{\sim}{x}_{K+1}\right)\left(\hat{\underset{\sim}{x}}_{K+1}^K - \underset{\sim}{x}_{K+1}\right)^T\right] \tag{4.21}$$

and represents the error in the predicted estimate $\hat{\underset{\sim}{x}}_{K+1}^K$ of $\underset{\sim}{x}_{K+1}$ at t_{K+1} based upon measurements up to and including $\underset{\sim}{y}_K$ at t_K and is given by

$$\underset{\sim}{P}_{K+1}^K = \underset{\sim}{\Phi}_{K+1}^K \underset{\sim}{P}_K^K \underset{\sim}{\Phi}_{K+1}^{K\ T} + \underset{\sim}{\Omega}_{K+1}, \tag{4.22}$$

$$P_0^0 \equiv M_0. \tag{4.23}$$

Note in equation (4.22) that Ω_{K+1} is the uncertainty in the estimate due to the stochastic input $w(t)$ acting over the interval $t_K \leq t < t_{K+1}$ in the state equation (4.1). This is discussed in Section 4.1.2 and at length in Appendix B. This is pointed out here since many references for the Kalman Filter assume a discrete form for the stochastic input which is sampled and held as in (4.13) and (4.16). In those cases, the so-called disturbance distribution matrix Γ_{K+1}^K in (4.16) comes into the predicted error covariance equation as follows:

$$P_{K+1}^K = \Phi_{K+1}^K P_K^K \Phi_{K+1}^{K\,T} + \Gamma_{K+1}^K W_K \Gamma_{K+1}^{K\,T},$$

where W_K is the sampled value of the disturbance covariance matrix $W(t)$ at $t = t_K$ in (4.3). In this thesis, since the system being studied is continuous in nature, equation (4.22) will be used instead.

The Kalman gain for the optimal filter may be shown to be

$$G_{K+1} = P_{K+1}^K C_{K+1}^T \left[C_{K+1} P_{K+1}^K C_{K+1}^T + V_{K+1} \right]^{-1}. \tag{4.24}$$

The predicted state estimate at time t_{K+1} knowing measurements at times up to and including t_K is

$$\hat{x}_{K+1}^K = \Phi_{K+1}^K \hat{x}_K^K + \psi_{K+1}^K u_K, \tag{4.25}$$

$$\hat{x}_0^0 \equiv m_0. \tag{4.26}$$

The corrected state estimate at t_{K+1} including the measurement at time t_{K+1} is

$$\hat{x}_{K+1}^{K+1} = \hat{x}_{K+1}^K + G_{K+1} \left[y_{K+1} - C_{K+1} \hat{x}_{K+1}^K \right]. \tag{4.27}$$

And finally, the corrected error covariance matrix at t_{K+1} given statistics of the measurement at t_{K+1} is

$$\underset{\sim}{P}_{K+1}^{K+1} = \left[\underset{\sim}{I} - \underset{\sim}{G}_{K+1}\underset{\sim}{C}_{K+1}\right]\underset{\sim}{P}_{K+1}^{K}\left[\underset{\sim}{I} - \underset{\sim}{G}_{K+1}\underset{\sim}{C}_{K+1}\right]^{T} + \underset{\sim}{G}_{K+1}\underset{\sim}{V}_{K+1}\underset{\sim}{G}_{K+1}^{T}. \quad (4.28)$$

An alternate form of the above can be shown to be

$$\underset{\sim}{P}_{K+1}^{K+1} = \left[\underset{\sim}{I} - \underset{\sim}{G}_{K+1}\underset{\sim}{C}_{K+1}\right]\underset{\sim}{P}_{K+1}^{K}. \quad (4.29)$$

Each form has its own advantages as will be shown in the next chapter.

Note the choices for the initial conditions for the covariance equation (4.23) and the state estimate (4.26). They are precisely those given for the system itself in (4.18). This is the best information available about the initial state to use in the filter. It turns out that if knowledge of these initial conditions is imprecise, the effect upon the later values of the state estimate diminishes as new measurements are processed.

4.2.2 Summary of Filter Algorithm — For convenience, the system simulation equations and Kalman Filter equations are listed together as in Figure 4.1.

The equations in Figure 4.1 are sufficient to both simulate a physical system((4.16) and (4.17)) when the actual system cannot be used, and to compute the filter calculations themselves. The computational cycle is as in the figure. Time is initialized to zero, K = 0, and each equation computed. Upon completion of one cycle, time is incremented and the recursion is carried out again until the final time of interest is reached.

$$\underset{\sim}{x}_{K+1} = \underset{\sim}{\Phi}^{K}_{K+1}\underset{\sim}{x}_{K} + \underset{\sim}{\Psi}^{K}_{K+1}\underset{\sim}{u}_{K} + \underset{\sim}{\Gamma}^{K}_{K+1}\underset{\sim}{w}_{K}, \qquad \underset{\sim}{x}_{0} \sim N(\underset{\sim}{m}_{0}, \underset{\sim}{M}_{0}) \tag{4.16}$$

$$\underset{\sim}{P}^{K}_{K+1} = \underset{\sim}{\Phi}^{K}_{K+1}\underset{\sim}{P}^{K}_{K}\underset{\sim}{\Phi}^{K}_{K+1}{}^{T} + \underset{\sim}{\Omega}_{K+1}, \qquad \underset{\sim}{P}^{0}_{0} = \underset{\sim}{M}_{0} \tag{4.22}$$

$$\underset{\sim}{G}_{K+1} = \underset{\sim}{P}^{K}_{K+1}\underset{\sim}{C}_{K+1}{}^{T}\left[\underset{\sim}{C}_{K+1}\underset{\sim}{P}^{K}_{K+1}\underset{\sim}{C}_{K+1}{}^{T} + \underset{\sim}{V}_{K+1}\right]^{-1} \tag{4.24}$$

$$\hat{\underset{\sim}{x}}^{K}_{K+1} = \underset{\sim}{\Phi}^{K}_{K+1}\hat{\underset{\sim}{x}}^{K}_{K} + \underset{\sim}{\Psi}^{K}_{K+1}\underset{\sim}{u}_{K}, \qquad \hat{\underset{\sim}{x}}^{0}_{0} = \underset{\sim}{m}_{0} \tag{4.25}$$

$$\underset{\sim}{y}_{K+1} = \underset{\sim}{C}_{K+1}\underset{\sim}{x}_{K+1} + \underset{\sim}{v}_{K+1} \tag{4.17}$$

$$\hat{\underset{\sim}{x}}^{K+1}_{K+1} = \hat{\underset{\sim}{x}}^{K}_{K+1} + \underset{\sim}{G}_{K+1}\left[\underset{\sim}{y}_{K+1} - \underset{\sim}{C}_{K+1}\hat{\underset{\sim}{x}}^{K}_{K+1}\right] \tag{4.27}$$

$$\underset{\sim}{P}^{K+1}_{K+1} = \left[\underset{\sim}{I} - \underset{\sim}{G}_{K+1}\underset{\sim}{C}_{K+1}\right]\underset{\sim}{P}^{K}_{K+1}\left[\underset{\sim}{I} - \underset{\sim}{G}_{K+1}\underset{\sim}{C}_{K+1}\right]^{T} + \underset{\sim}{G}_{K+1}\underset{\sim}{V}_{K+1}\underset{\sim}{G}_{K+1}{}^{T} \tag{4.28}$$

Figure 4.1. System simulation and Kalman Filter computation.

CHAPTER 5. OPTIMAL DESIGN AND MANAGEMENT OF MONITORING SYSTEMS

The purpose of this chapter is to propose a method of solution for the monitoring problem as stated in Chapter 2. The models for various processes considered in Chapter 3 are discretized using the methods of Chapter 4 for computation in the Kalman Filter. The structure of the filter is studied in the context of the monitoring problem in order to obtain a set of monitoring design and managment equations. Properties of these equations are examined in detail to yield the optimal solution for the monitoring problem for the case of time-invariant systems with constant source and measurement noise statistics and time-invariant estimation accuracy constraint. Numerical examples to illustrate the conclusions follow in Chapter 6.

5.1 Monitoring and the Kalman Filter

As stated in Chapter 2, two variations of the monitoring problem arise in practice. The first is to maintain the error in the estimate of the state of the system below some bound over the complete time interval of interest. The emphasis on limiting the error in the estimate of the state arises in the use of that estimate in closed-loop state feedback applications where high accuracy in the state estimate is of primary importance. The second variation in the monitoring problem is to maintain the error in the estimate of the output, the system variable itself, everywhere in the medium, below some bound throughout the time interval of interest. The system variable could be pollutant concentration, radiation level, temperature, etc. The thrust behind maintaining high

accuracy in the knowledge of the system variable comes with application in the detection problem, where it is required to know, to some degree of certainty, where and when a pollutant concentration exceeds a legal limit.

Both of these variants can be approached within the structure of the Kalman Filter. As described in Chapter 4, the filter provides an optimal estimate of the state of a linear, stochastic process, optimal in the sense that the expected mean-square error between the estimate and the state itself is minimized. Thus, when taking a measurement of an actual physical system, the Kalman Filter uses the information obtained in the measurement in the best way in order to update the estimate of the state. The discrete-time, recursive nature of the filter provides a fertile structure from which the solution to the monitoring problem can grow.

In either case, with a bound on state or output estimate error, the basic structure of the problem is the same; to take the fewest total number of samples over a given time interval in order to maintain the error in the estimate within some bound. This says nothing about the number of samples to be made at each measurement time, whether or not that number changes from measurement to measurement, whether sample locations move from measurement to measurement, just that when the time interval is over, the least number of samples were necessary to insure the accuracy of the estimate.

As summarized in Figure 4.1, the first step in the Kalman Filter algorithm is to initialize the estimate of the state vector and state estimate error covariance matrix (from (4.26) and (4.23)). The state estimate and its error covariance matrix are then predicted ahead one

step in time ((4.16) and (4.22)). Before each measurement, the Kalman gain is computed (4.24). Next a measurement is made of the process itself (4.17) which starts the correction phase of the algorithm. The new information from that measurement is used to correct the estimate of the state (4.27) and the statistics associated with the measurement are used to correct the error covariance matrix (4.28). Finally, the time is incremented and the new corrected values are used to reinitialize the prediction equations at the beginning of the algorithm so that the algorithm may be repeated for the next cycle.

This sequence of predicting, taking a measurement, correcting, predicting, taking another measurement, etc., was the original calculational form of the Kalman Filter (see Kalman [66]). Since then, applications to guidance and orbit determination, for example, have resulted in splitting apart the prediction and correction phases, allowing for recursive prediction of many cycles before a measurement is taken and its corresponding correction made [30], [44], [65]. Moore [95] has shown how this splitting applies in use of the Extended Kalman Filter in monitoring system design for nonlinear aquatic ecosystems (see Jazwinski [65] for detailed discussion of the Extended Kalman Filter). Thus, separating the prediction and correction of the estimate has been suggested as a beginning for the solution to the optimal monitoring system design and management problems (see Brewer and Moore [24] and Brewer and Hubbard [23]).

Suppose then, that the Kalman Filter algorithm is initialized as usual but instead of taking measurements at each cycle, sampling is deferred until it is absolutely necessary to gain more information about the actual system through a measurement in order to maintain the error in the estimate within some bound. This seems like an approach which

would logically lead to the fewest number of samples over a given time interval but in fact, the optimality of sampling only at times when the error limit is reached is difficult to prove. Since it can be shown that for certain special cases, the minimum cost measurement program is to sample *only* when the estimation error is at its limit, assume for now that the optimality of such a sampling schedule extends to all cases in order to proceed in the development of relationships for the optimal design problem; defer until later proof of the fact that sampling at the limit is the optimal solution of the management problem.

Once the bound is reached, it is necessary to take a measurement. A major phase in the monitoring problem is at hand, that referred to as the "design" problem [24]. At a measurement time, the design problem seeks to answer the following questions:

1) What is the best number of samples to take for this measurement;
2) What are the best types of samplers to deploy;
3) Where are the best sites in the medium at which to locate the samplers?

The term "best" appears in all these questions but best is what sense? In the context of the monitoring problem here posed, best can *only* mean in the manner which will lead to the fewest total number of samples being taken over the entire time interval of interest. Thus, if the assumption of the previous paragraph is true, that is, if it is optimal to sample at the estimate error limit only, then the goal of the design problem should simply be to answer (1), (2), and (3) above such that the *time* when the error bound is next reached is *maximized*. Then, if at each measurement, the time to the next measurement is maximized, overall, the number of measurement times should be minimized.

However, this does not take into account changing numbers of samplers at various measurements. For now, ignore this part of the problem in order to establish firm results about the case where the same number of samplers are used at each measurement time, deferring until later remarks about the general problem.

Thus, the result in the solution of the "design" problem also solves the "management" problem, that of the optimal timing of the measurements. With this framework established for solution of the monitoring problem, first the case of bound on error in the state estimate is considered, then that of bound on error in the estimate of the system variable, or output, will be dealt with.

5.2 One-Dimensional Diffusion with No-Flow Boundary Conditions

A most important recent application of normal mode analysis is the bilateral coupling of diffusive elements (see Young [131]). Through simplifying infinite order normal mode models in a quantitative manner, it is possible to approximate the characteristics of an inhomogeneous medium by coupling together homogeneous models. This is done by assuming "no-flow" or Neumann boundary conditions at the junctions and introducing pseudo-sources to account for resultant differences. The technique readily extends to multiple space dimensions and is thus, very powerful.

With the practical importance of this technique established [131], the case of one-dimensional diffusion with no-flow boundary conditions is a fundamental system to consider in optimal monitoring system design and management. This case is used as the basis for all the theoretical developments in the following sections. For completeness, extensions and applications of the results to other diffusive systems are considered in the last sections of this chapter.

5.3 The Design Problem for a Bound on the Error in the State Estimate

5.3.1 The Infrequent Sampling Problem — In the statement of the recursive linear estimation problem in Chapter 4, the Kalman Filter was stated to be that filter which minimizes the mean-square length of the error vector between the estimate of the state and the state itself of a linear stochastic system. That is, for all times, t_K, it minimizes

$$E\left[\left(\hat{\underset{\sim}{x}}_K - \underset{\sim}{x}_K\right)^T\left(\hat{\underset{\sim}{x}}_K - \underset{\sim}{x}_K\right)\right]. \tag{4.20}$$

Notice, from (4.20) and (4.29) that the covariance matrix is defined by

$$E\left[\left(\hat{\underset{\sim}{x}}_{K+1} - \underset{\sim}{x}_{K+1}\right)\left(\hat{\underset{\sim}{x}}_{K+1} - \underset{\sim}{x}_{K+1}\right)^T\right] \equiv \underset{\sim}{P}^{K+1}_{K+1}, \tag{5.1}$$

that is, at time t_{K+1}, the covariance matrix just after the sample is given by $\underset{\sim}{P}^{K+1}_{K+1}$. It can be seen from the above that

$$E\left[\left(\hat{\underset{\sim}{x}}_{K+1} - \underset{\sim}{x}_{K+1}\right)^T\left(\hat{\underset{\sim}{x}}_{K+1} - \underset{\sim}{x}_{K+1}\right)\right] = \mathrm{Tr}\left[\underset{\sim}{P}^{K+1}_{K+1}\right]. \tag{5.2}$$

Thus, in order to minimize the mean-square length of the estimation error vector for a measurement at time t_{K+1}, that measurement should be chosen which minimizes the trace of the corrected covariance matrix. Thus, the choice of a convenient scalar performance index for the problem of maintaining the error in the *state* estimate within some bound is to use the *trace* of the estimation error covariance matrix.

Returning then to the requirements of the design strategy of the last section, it is necessary to choose a measurement so that, in this case, *the time when the trace* of the covariance matrix *next reaches its limit* will be *maximized*. This might be thought to be the same thing as finding that measurement which minimizes the trace of the covariance matrix *at the time of the measurement*; but as will be seen, these are not necessarily equivalent. To study the evolution in time of the

trace of the covariance matrix, repeat the equations for the predicted and corrected covariance matrices:

$$\underset{\sim}{P}^{K}_{K+1} = \underset{\sim}{\Phi}^{K}_{K+1}\underset{\sim}{P}^{K}_{K}\underset{\sim}{\Phi}^{K}_{K+1}{}^{T} + \underset{\sim}{\Omega}_{K+1}, \tag{4.22}$$

$$\underset{\sim}{P}^{K+1}_{K+1} = \left[\underset{\sim}{I} - \underset{\sim}{G}_{K+1}\underset{\sim}{C}_{K+1}\right]\underset{\sim}{P}^{K}_{K+1}\left[\underset{\sim}{I} - \underset{\sim}{G}_{K+1}\underset{\sim}{C}_{K+1}\right]^{T} + \underset{\sim}{G}_{K+1}\underset{\sim}{V}_{K+1}\underset{\sim}{G}_{K+1}{}^{T}, \tag{4.28}$$

where

$$\underset{\sim}{G}_{K+1} = \underset{\sim}{P}^{K}_{K+1}\underset{\sim}{C}_{K+1}{}^{T}\left[\underset{\sim}{C}_{K+1}\underset{\sim}{P}^{K}_{K+1}\underset{\sim}{C}_{K+1}{}^{T} + \underset{\sim}{V}_{K+1}\right]^{-1} \tag{4.24}$$

Use (4.24) and (4.29) to obtain

$$\underset{\sim}{P}^{K+1}_{K+1} = \underset{\sim}{P}^{K}_{K+1} - \underset{\sim}{P}^{K}_{K+1}\underset{\sim}{C}_{K+1}{}^{T}\left[\underset{\sim}{C}_{K+1}\underset{\sim}{P}^{K}_{K+1}\underset{\sim}{C}_{K+1}{}^{T} + \underset{\sim}{V}_{K+1}\right]^{-1}\underset{\sim}{C}_{K+1}\underset{\sim}{P}^{K}_{K+1}. \tag{5.3}$$

Note that the two forms for $\underset{\sim}{P}^{K+1}_{K+1}$, (4.28) and (5.3), can be shown to be equivalent (see Sorensen [78]) Both are listed since it is well-known that the former is superior computationally from an accuracy point of view in that it tends to preserve the positive-definiteness of the covariance matrices better (see Aoki [3],) but the latter is much simpler to manipulate analytically. Thus, (5.3) will be used in all the analysis involved in the solution of the monitoring problem and in any numerical gradient algorithms resulting from that analysis whereas (4.28) will be used directly in the filter calculations themselves.

To make the problem tractable, constrain the range of the problem as follows:

> *Assumption: Only systems of the form (3.40) will be considered where the system matrix $\underset{\sim}{A}$, control matrix $\underset{\sim}{B}$ and disturbance matrix $\underset{\sim}{D}$ are all <u>time-invariant</u> and where the disturbance noise covariance matrix $\underset{\sim}{W}$ and measurement noise covariance matrix $\underset{\sim}{V}$ are <u>constant</u>.* (5.4)

With this assumption, initialize the algorithm at time t_0 by setting the covariance matrix in (4.22) to $\underset{\sim}{M}_0$. Then, predict to time t_1 to get

$$\underset{\sim}{P}^{0}_{1} = \underset{\sim}{\Phi}\underset{\sim}{M}_0\underset{\sim}{\Phi}^{T} + \underset{\sim}{\Omega}, \tag{5.5}$$

where the subscripts have been dropped owing to the condition of assumption (5.4) and $\underset{\sim}{\Phi}$ for a fixed time step is given in (4.9). Next, it is necessary to check to see if the error limit which may be called Tr_{lim} has been reached. That is, is

$$Tr\left[\underset{\sim}{P}_1^0\right] \geq Tr_{lim} \ ?$$

If not, advance in time to t_2 and predict ahead again:

$$\begin{aligned}\underset{\sim}{P}_2^0 &= \underset{\sim}{\Phi}\underset{\sim}{P}_1^0\underset{\sim}{\Phi}^T + \underset{\sim}{\Omega} \\ &= \underset{\sim}{\Phi}^2\underset{\sim}{M}_0\underset{\sim}{\Phi}^{2T} + \underset{\sim}{\Phi}\underset{\sim}{\Omega}\underset{\sim}{\Phi}^T + \underset{\sim}{\Omega}. \end{aligned} \tag{5.6}$$

Check again:

$$Tr\left[\underset{\sim}{P}_2^0\right] \geq Tr_{lim} \ ?$$

If not,

$$\begin{aligned}\underset{\sim}{P}_3^0 &= \underset{\sim}{\Phi}\underset{\sim}{P}_2^0\underset{\sim}{\Phi}^T + \underset{\sim}{\Omega} \\ &= \underset{\sim}{\Phi}^2\underset{\sim}{P}_1^0\underset{\sim}{\Phi}^{2T} + \underset{\sim}{\Phi}\underset{\sim}{\Omega}\underset{\sim}{\Phi}^T + \underset{\sim}{\Omega} \\ &= \underset{\sim}{\Phi}^3\underset{\sim}{M}_0\underset{\sim}{\Phi}^{3T} + \underset{\sim}{\Phi}^2\underset{\sim}{\Omega}\underset{\sim}{\Phi}^{2T} + \underset{\sim}{\Phi}\underset{\sim}{\Omega}\underset{\sim}{\Phi}^T + \underset{\sim}{\Omega}. \end{aligned} \tag{5.7}$$

Assume that after K steps, the limit is finally reached. From Appendix C, (5.7) can be generalized to the form

$$\underset{\sim}{P}_K^0 = \underset{\sim}{\Phi}^K\underset{\sim}{M}_0\underset{\sim}{\Phi}^{KT} + \sum_{n=1}^{K} \underset{\sim}{\Phi}^{n-1}\underset{\sim}{\Omega}\underset{\sim}{\Phi}^{n-1T}. \tag{5.8}$$

It is now necessary to make a measurement. Apply (5.3) to obtain, for the measurement at time t_K,

$$\underset{\sim}{P}_K^K = \underset{\sim}{P}_K^0 - \underset{\sim}{P}_K^0\underset{\sim}{C}_K^T\left[\underset{\sim}{C}_K\underset{\sim}{P}_K^0\underset{\sim}{C}_K^T + \underset{\sim}{V}\right]^{-1}\underset{\sim}{C}_K\underset{\sim}{P}_K^0. \tag{5.9}$$

Note here that from assumption (5.4), $\underset{\sim}{V}$ is a constant, thus no subscripts, but $\underset{\sim}{C}_K$ is *not*. $\underset{\sim}{C}_K$ is what is available to change in the design of the

measurement to be taken. It is again, to be chosen to maximize the time over which prediction may take place before the limit on the trace of the predicted covariance matrix is reached at the next measurement. That is, find $\underline{C}_K$ at time t_K such that N is maximized where

$$\underline{P}^K_{K+N} = \underline{\Phi}^N \underline{P}_K \underline{\Phi}^{N^T} + \sum_{n=1}^{N} \underline{\Phi}^{n-1} \underline{\Omega} \underline{\Phi}^{n-1^T}, \tag{5.10}$$

and

$$\mathrm{Tr}\left[\underline{P}^K_{K+N}\right] \geq \mathrm{Tr}_{\ell i m}. \tag{5.11}$$

In developing a strategy for the choice of $\underline{C}_K$ to maximize N, the properties of (5.10), the matrix solution of the linear matrix recurrence (4.22), are now considered. Since the recurrence is linear in $\underline{P}$, its solution may be decomposed into the zero-input response and the zero-state response; these terms are more commonly known as the homogeneous or unforced and particular or forced solutions in differential equations or dynamic system theory. The first term in (5.10) is seen to involve only the initial "state" of the covariance matrix just after the sample at time t_K, the zero-input response. The second term, the zero-state response, has nothing to do with the covariance at time t_K and involves only the strength of the disturbance noise, $\underline{\Omega}$. An observation can thus already be stated:

> Conclusion I. The selection of $\underline{C}_K$ at time t_K to maximize t_{K+N}, the time of the next measurement, is solely a function of $\underline{P}^K_K$ and not the forcing function. (C.I)

This can be seen by rewriting (5.10) as follows:

$$P^{K}_{K+N}(C_K) = \Phi^N P^K_K(C_K)\Phi^{N^T} + \sum_{n=1}^{N} \Phi^{n-1}\Omega\Phi^{n-1^T}. \qquad (5.12)$$

Here, it is seen that the predicted value of the covariance matrix at time t_{K+N} is a function of the measurement matrix *back at time* t_K. However, only the first of the two terms in the expression for the predicted covariance matrix involves that measurement matrix.

Thus, in order for t_{K+N} to be as large as possible before condition (5.11) is met, it is required that the trace of the covariance matrix *at time* t_{K+N} be *minimized* by the appropriate choice of the measurement matrix *at time* t_K. This presents a formidable problem in the general case. The general solution might be approached through the use of dynamic programming or through a direct search algorithm structured as follows:

(1) Pick, in some manner, C_{K_i};
(2) Predict ahead to time t_{K+N} using (5.12) until
(3) $Tr[P^K_{K+N}(C_{K_i})] \geq Tr_{lim}$
(4) Store N in N_i, return to (1);
(5) Stop when convergence to largest possible N_i is assured. (5.13)

Such a procedure could be quite costly to execute since it is a direct search technique, rather than a technique for which an analytical expression for the gradient of the objective function can be found. Also, each evaluation of the objective function, that is, the finding of each N_i when (3) is satisfied, involves carrying out the solution of the matrix equation (4.22) N_i times (it should be mentioned that since the interest here is only in the trace, only the diagonal terms of (4.22) need be computed each time, but this is still costly, nonetheless).

Since an algorithm of the type in (5.13) is cumbersome at best, seek more concise solutions for the problem in (5.10) and (5.11). To do

this, more information on the structure of the process involved is necessary, that is, more knowledge of the forms of $\underset{\sim}{\Phi}$ and $\underset{\sim}{\Omega}$. Suppose the system which $\underset{\sim}{\Phi}$ represents is a one-dimensional diffusion process with no-flow boundary conditions: see Section 3.2.1 for such a system. Suppose that the problem is formulated in normal modes so that the system matrix, from (3.37), is given as

$$\underset{\sim}{A} \equiv \begin{bmatrix} 0 & & \bigcirc \\ & -\frac{K\pi^2}{4L^2} & \\ & & \ddots \\ \bigcirc & & -(n-1)^2\frac{K\pi^2}{4L^2} \end{bmatrix} \tag{5.14}$$

Thus, for this time-invariant system matrix, its state transition matrix for the time step $T \equiv (t_{K+1} - t_K)$ according to (4.9) is given by

$$\underset{\sim}{\Phi} \equiv e^{\underset{\sim}{A}T} = \begin{bmatrix} 1 & & \bigcirc \\ & e^{-\frac{K\pi^2}{4L^2}T} & \\ & & \ddots \\ \bigcirc & & e^{-(n-1)^2\frac{K\pi^2}{4L^2}T} \end{bmatrix}. \tag{5.15}$$

Notice that with the ordering of the eigenvalues in the system matrix in (5.14), the diagonal elements of $\underset{\sim}{\Phi}$, written ϕ_{ii}, exhibit the following property:

$$\phi_{11} = 1; \qquad \phi_{ii} > \phi_{i+1,i+1} > 0, \quad i = 1,2,3,\ldots,n-1, \tag{5.16}$$

where n is the number of states retained in the normal mode mode and is thus also the dimension of the square matrices $\underset{\sim}{A}$ and $\underset{\sim}{\Phi}$. Choice of

a normal mode model has resulted in this unique relationship in (5.16) which allows drastic simplification of the optimization problem in (5.10) and (5.11).

Expand equation (5.10) to obtain

$$P^K_{K\bullet N} = \begin{bmatrix} \left[P^K_K\right]_{11} & \left[P^K_K\right]_{12}\phi^N_{11}\phi^N_{22} & \left[P^K_K\right]_{13}\phi^N_{11}\phi^N_{33} & \cdots \\ \left[P^K_K\right]_{21}\phi^N_{22}\phi^N_{11} & \left[P^K_K\right]_{22}\phi^{2N}_{22} & & \\ \vdots & \vdots & & \\ & & & \left[P^K_K\right]_{rrr}\phi^{2N}_{rrr} \end{bmatrix}$$

$$+ \begin{bmatrix} N[Q]_{11} & [Q]_{12}\sum_{n=1}^{N}\phi^{n-1}_{11}\phi^{n-1}_{22} & [Q]_{13}\sum_{n=1}^{N}\phi^{n-1}_{11}\phi^{n-1}_{33} & \cdots \\ [Q]_{21}\sum_{n=1}^{N}\phi^{n-1}_{22}\phi^{n-1}_{11} & [Q]_{22}\sum_{n=1}^{N}\phi^{2(n-1)}_{22} & \cdots & \\ \vdots & \vdots & & \\ & & & [Q]_{rrr}\sum_{n=1}^{N}\phi^{2(n-1)}_{rrr} \end{bmatrix}. \tag{5.17}$$

From the form of (5.17), using property (5.16) shows that for N large, the first term of (5.10) is given by

$$\lim_{N\to\infty}\left[\Phi^N P^K_{K\bullet} \Phi^{N^T}\right]_{ij} = \begin{cases} \left[P^K_K\right]_{11}; & i = 1,\ j = 1 \\ 0 \quad ; & i \text{ and } j \neq 1, \end{cases} \tag{5.18}$$

Thus, for N sufficiently large, all that is left of the homogeneous term in (5.10) at time t_{K+N} is the first element of $\underline{P}_K^K$ at time t_K. This result, together with Conclusion I yields

Conclusion II. For N large, the following are equivalent:
(1) Find $\underline{C}_K$ which minimizes $Tr\left[\underline{P}_{K+N}^K(\underline{C}_K)\right]$;
(2) Find $\underline{C}_K$ which minimizes $\left[\underline{P}_K^K(\underline{C}_K)\right]_{11}$. (C.II)

From the discussion just after (5.12) it is obvious now that the choice of $\underline{C}_K^*$, for the optimal measurement matrix at time t_K, can be stated as

Conclusion III. For N large, to maximize t_{K+N}, the time when $Tr\left[\underline{P}_{K+N}^K(\underline{C}_K)\right] \geq Tr_{lim}$, choose $\underline{C}_K^*$ at time t_K which minimizes $\left[\underline{P}_K^K(\underline{C}_K)\right]_{11}$. (C.III)

Thus, for the asymptotic case of N sufficiently large so that (5.18) applies within some tolerance level, the monitoring problem is solved. Such an infrequent sampling program may well apply to many physical systems where the dynamics of the transient response are fast in comparison to the time between samples. The above conclusions reduce the monitoring system design problem to one of minimization of the (1,1)-element of $\underline{P}_K^K$ in (5.9), a procedure for which writing the gradient of the objective function is straightforward.

In order to more fully understand the nature of the solution (5.10), consider the second term, the zero-state response, in (5.10) and (5.17). This term is a matrix convolution of the disturbance covariance matrix $\underline{\Omega}$ and the state transition matrix $\underline{\phi}$. As such, it possesses qualities of convolutions of other linear processes. Write the general element for the second term of (5.17) as

$$\Omega_{Nij} \equiv [\underline{\Omega}]_{ij} \sum_{n=1}^{N} \phi_{ii}^{n-1}\phi_{jj}^{n-1}, \qquad i \text{ and } j \neq 1. \tag{5.19}$$

From property (5.16), $0 \leq \phi_{ii} < 1$, $i \neq 1$. Recognizing the products $(\phi_{ii}\phi_{jj})$ in the convolution term in (5.17) as common ratios in geometric progressions, the element of the matrix convolution may be seen to approach the limit

$$\left[\underset{\sim}{\Omega}_{SS}\right]_{ij} \equiv \lim_{N\to\infty} [\underset{\sim}{\Omega}]_{ij} \sum_{n=1}^{N} \phi_{ii}^{n-1}\phi_{jj}^{n-1} = \lim_{N\to\infty} [\underset{\sim}{\Omega}]_{ij} \left\{\frac{1-(\phi_{ii}\phi_{jj})^{N}}{1-\phi_{ii}\phi_{jj}}\right\} = \frac{[\underset{\sim}{\Omega}]_{ij}}{1-\phi_{ii}\phi_{jj}}, \quad i \text{ and } j \neq 1. \tag{5.20}$$

Thus, all the elements in the second term of (5.17) go to steady-state constants as N gets large, except the first which grows monotonically as a ramp with slope $[\underset{\sim}{\Omega}]_{11}$.

Thus, (5.10) may be written schematically as

$$\begin{bmatrix} \\ \underset{\sim}{P}^{K}_{K+N} \\ \\ \end{bmatrix} = \begin{bmatrix} \left[\underset{\sim}{P}^{K}_{K}\right]_{11} & \\ & \bigcirc \end{bmatrix} + \begin{bmatrix} N[\underset{\sim}{\Omega}]_{11} & \\ & \bigcirc \end{bmatrix} + \begin{bmatrix} 0 & \\ & \underset{\sim}{\Omega}_{SS} \end{bmatrix} \tag{5.21}$$

where the (1,1)-elements of the matrices are shown partitioned from all the other elements of those matrices; this is a notational convenience used throughout what follows.

From (5.21), the simplified relationship for the trace can be written as

$$\mathrm{Tr}\left[\underset{\sim}{P}^{K}_{K+N}(\underset{\sim}{C}_{K})\right] \simeq \left[\underset{\sim}{P}^{K}_{K}(\underset{\sim}{C}_{K})\right]_{11} + N[\underset{\sim}{\Omega}]_{11} + \mathrm{Tr}\left[\underset{\sim}{\Omega}_{SS}\right]. \tag{5.22}$$

The meaning of Conclusion II becomes clear in that changing the nature of the measurement at time t_K by changing $\underset{\sim}{C}_K$ effects the value of $\mathrm{Tr}\left[\underset{\sim}{P}^{K}_{K+N}(\underset{\sim}{C}_K)\right]$ only through $\left[\underset{\sim}{P}^{K}_{K}(\underset{\sim}{C}_K)\right]_{11}$ for N sufficiently large. Also, say the equality in (5.11) is just met at time t_{K+N}. Then,

$$\mathrm{Tr}\left[\underset{\sim}{P}^{K}_{K+N}(\underset{\sim}{C}_{K})\right] = \mathrm{Tr}_{lim} \simeq \left[\underset{\sim}{P}^{K}_{K}(\underset{\sim}{C}_{K})\right]_{11} + N[\underset{\sim}{\Omega}]_{11} + \mathrm{Tr}\left[\underset{\sim}{\Omega}_{SS}\right]. \tag{5.23}$$

(5.23) can be used to demonstrate Conclusion III. From (5.20) and with

$\underset{\sim}{\Omega}_{SS}$ as defined in (5.21), it is seen that for various choices of $\underset{\sim}{C}_K$ in (5.23), $Tr\left[\underset{\sim}{\Omega}_{SS}\right]$ remains invariant so long as N remains sufficiently large. Thus, in the equality in (5.23), the first two terms on the right-hand side always sum to a constant and as $\underset{\sim}{C}_K$ is chosen to minimize $\left[\underset{\sim}{P}^K_K(\underset{\sim}{C}_K)\right]_{11}$, N in the second term is maximized; Conclusion III is thus seen to hold whenever the limit in (5.18) is approached.

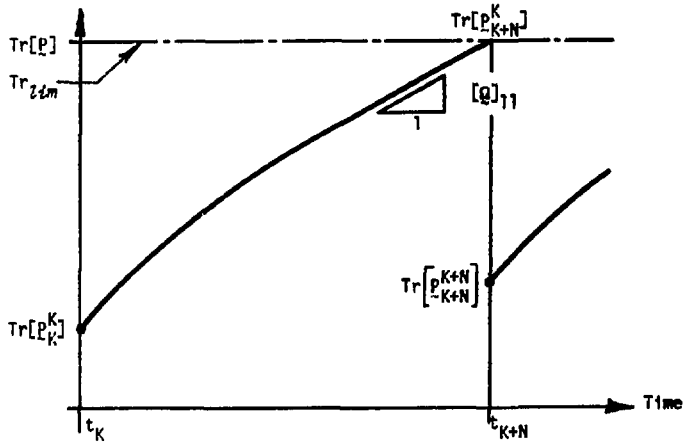
A graphical depiction of the relationships in (5.22) and (5.23) is shown in Figure 5.1. In Figure 5.1A, a representation of a typical plot of the full trace of $\underset{\sim}{P}$ over time is shown while in Figure 5.1B, the elements of the asymptotic approximation in (5.22) are drawn. Writing the trace of the matrices in (5.17), obtain

$$Tr\left[\underset{\sim}{P}^K_{K+N}\right] = \left(\left[\underset{\sim}{P}^K_K\right]_{11} + \left[\underset{\sim}{P}^K_K\right]_{22}\phi_{22}^{2N} + \ldots + \left[\underset{\sim}{P}^K_K\right]_{nn}\phi_{nn}^{2N}\right) + \left(N[\underset{\sim}{\Omega}]_{11} + [\underset{\sim}{\Omega}]_{22}\sum_{n=1}^{N}\phi_{22}^{2(n-1)} + \ldots + [\underset{\sim}{\Omega}]_{nn}\sum_{n=1}^{N}\phi_{nn}^{2(n-1)}\right). \quad (5.24)$$

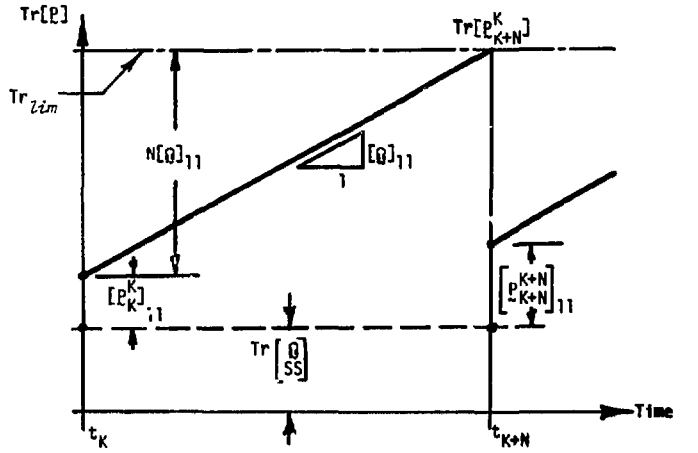
As N grows large, (5.24) tends to (5.22) but during the initial transient period, the last terms of both lines of (5.24) are going through changes. These changes account for the approach to the asymptotic slope near time t_K in Figure 5.1A.

Notice how if a different choice of $\underset{\sim}{C}_K$ results in a smaller value of $\left[\underset{\sim}{P}^K_K(\underset{\sim}{C}_K)\right]_{11}$ in Figure 5.1B, that the start of the plot would be translated downward with the same offset of $Tr[\underset{\sim}{\Omega}_{SS}]$ to result in a *longer* time interval before the limit Tr_{lim} is reached again.

5.3.2 The Effect of *a priori* Statistics — Choice of $\underset{\sim}{M}_0$ and $\underset{\sim}{m}_0$ in the filter equations (4.16) and (4.22) has come under considerable study ever since the introduction of the Kalman Filter. Much effort has gone into identifying these terms in actual applications and consider-



(A) Actual response



(B) Asymptotic approximation

Figure 5.1. Schematic representation of the basic relationships in the infrequent sampling problem.

able time spent in assessing the sensitivity of the results to lack of knowledge of the initial statistics. Attention is now turned to these topics within the framework of the above results for the case of infrequent sampling.

It is required to find the effects that various values for $\underset{\sim}{M}_0$, the matrix of initial uncertainties in the estimate of the state, $\hat{\underset{\sim}{x}}_0^0$, have upon the optimal measurement system design $\underset{\sim}{C}_K^*$ for the first measurement at time t_K. For the case of bound on error in the state estimate, from (5.8), it is necessary to sample when

$$\mathrm{Tr}\left[\underset{\sim}{P}_K^0\right] = \mathrm{Tr}\left[\underset{\sim}{\Phi}^K \underset{\sim}{M}_0 \underset{\sim}{\Phi}^{K^T} + \sum_{n=1}^{K} \underset{\sim}{\Phi}^{n-1} \underset{\sim}{\Omega} \underset{\sim}{\Phi}^{n-1^T}\right] \geq \mathrm{Tr}_{lim}. \tag{5.25}$$

If K is sufficiently large at the first sample so that (5.18) approximately applies, then (5.25) may be written as

$$\left[\underset{\sim}{M}_0\right]_{11} + K[\underset{\sim}{\Omega}]_{11} + \mathrm{Tr}[\underset{SS}{\Omega}] \geq \mathrm{Tr}_{lim} \tag{5.26}$$

as in (5.23). Thus, only the (1,1)-element of matrix $\underset{\sim}{M}_0$ is of any significance in the first sample for K sufficiently large. Furthermore, since $\mathrm{Tr}[\underset{SS}{\Omega}]$ is a constant for various choices of $\underset{\sim}{M}_0$, the remaining two terms in the left-hand expression of (5.26) sum to a constant over all choices of $\underset{\sim}{M}_0$. To deduce the significance of this, write out the matrices for (5.25) in a manner similar to (5.21):

$$\underset{\sim}{P}_K^0 = \underset{\sim}{\Phi}^K \underset{\sim}{M}_0 \underset{\sim}{\Phi}^{K^T} + \sum_{n=1}^{K} \underset{\sim}{\Phi}^{n-1} \underset{\sim}{\Omega} \underset{\sim}{\Phi}^{n-1^T}; \tag{5.27}$$

for K large, (5.18) allows (5.27) to be written as

$$\begin{bmatrix} \\ \underset{\sim}{P}_K^0 \\ \\ \end{bmatrix} \simeq \begin{bmatrix} [\underset{\sim}{M}_0]_{11} & \\ & \mathcal{O} \end{bmatrix} + \begin{bmatrix} K[\underset{\sim}{\Omega}]_{11} & \\ & \mathcal{O} \end{bmatrix} + \begin{bmatrix} 0 & \\ & \underset{SS}{\Omega} \end{bmatrix}. \tag{5.28}$$

Note that if (5.20) applies, then a particularly important result follows, namely that the (1,1)-element of the predicted covariance matrix at the first measurement time is given by

$$\left[\underset{\sim}{P}_K^0\right]_{11} \simeq \left([\underset{\sim}{M}_0]_{11} + K[\underset{\sim}{\Omega}]_{11}\right) = \text{const}, \tag{5.29}$$

no matter what $\underset{\sim}{M}_0$ may be.

For the measurement itself, $\underset{\sim}{P}_K^0$ *is used in the following expression:*

$$\underset{\sim}{P}_K^K = \underset{\sim}{P}_K^0 - \underset{\sim}{P}_K^0 \underset{\sim}{C}_K^T \left[\underset{\sim}{C}_K \underset{\sim}{P}_K^0 \underset{\sim}{C}_K^T + \underset{\sim}{V}\right]^{-1} \underset{\sim}{C}_K \underset{\sim}{P}_K^0. \tag{5.30}$$

But from (5.28), since, for K large, $\underset{SS}{\Omega}$ is fixed, and since (5.29) holds, making the optimum choice $\underset{\sim}{C}_K^*$ of $\underset{\sim}{C}_K$ in (5.30) is independent of the initial error covariance matrix $\underset{\sim}{M}_0$, but directly related to Tr_{lim} which is summarized in the following:

> Conclusion IV. For K large, determination of the optimum measurement matrix $\underset{\sim}{C}_K^*$ at t_K is determined by the error limit Tr_{lim} and is independent of $\underset{\sim}{M}_0$. (C.IV)
>
> Conclusion V. For K large, the only effect $\underset{\sim}{M}_0$ has upon the monitoring program is in determining with Tr_{lim} the time of the first measurement t_K. (C.V)

Thus, if the constraint Tr_{lim} in (5.25) is such that (5.18) and thus (5.26) hold, choice of the initial condition for $\underset{\sim}{M}_0$ is of little importance. However, in practical applications, the better approach to the identification of the *a priori* statistics is to concentrate analytical efforts upon the identification of only the (1,1)-element of $\underset{\sim}{M}_0$ and not upon identifying the full matrix in cases where the simplifying approximations of the infrequent sampling problem apply. In this manner, a better estimate of the first state should be possible for the same

analytical effort leading to a longer time before the first sample is necessary.

5.3.3 Fixed Number of Samplers at Each Measurement and Fixed Error Limit — Thus far, little has been said about the number of sampling devices to be deployed at each measurement time. Consider here what happens when the same number of samplers, m, is to be used at each measurement. Consider further the case when the error limit placed upon the uncertainty in the state estimate, Tr_{lim}, is the same throughout the problem.

Suppose a sample has just been made at time t_K. In order to study the optimal designs which arise at different measurement times, consider the next two samples which occur at times t_{K+N_1} and $t_{K+N_1+N_2}$. Since Tr_{lim} is constant, if both N_1 and N_2 are large in the sense of (5.18), obtain the following conditions at the two sample times:

$$Tr\left[\underset{\sim}{P}^{K}_{K+N_1}\right] \simeq \left[\underset{\sim}{P}^{K}_{K}\left(\underset{\sim}{C}^{*}_{K}\right)\right]_{11} + N_1[\underset{\sim}{Q}]_{11} + Tr[\underset{SS}{\underset{\sim}{Q}}] \geq Tr_{lim}, \tag{5.31}$$

$$Tr\left[\underset{\sim}{P}^{K+N_1}_{K+N_1+N_2}\right] \simeq \left[\underset{\sim}{P}^{K+N_1}_{K+N_1}\left(\underset{\sim}{C}^{*}_{K+N_1}\right)\right]_{11} + N_2[\underset{\sim}{Q}]_{11} + Tr[\underset{SS}{\underset{\sim}{Q}}] \geq Tr_{lim}, \tag{5.32}$$

Since $Tr[\underset{SS}{\underset{\sim}{Q}}]$ is the same for both measurements, for the case of the equality in both (5.31) and (5.32), it is seen that

$$\left[\underset{\sim}{P}^{K}_{K}\left(\underset{\sim}{C}^{*}_{K}\right)\right]_{11} + N_1[\underset{\sim}{Q}]_{11} = \left[\underset{\sim}{P}^{K+N_1}_{K+N_1}\left(\underset{\sim}{C}^{*}_{K+N_1}\right)\right]_{11} + N_2[\underset{\sim}{Q}]_{11}. \tag{5.33}$$

Now, if the full matrices in (5.32) are written out, obtain

$$\begin{bmatrix} & \\ \underset{\sim}{P}^{K+N_1}_{K+N_1+N_2} & \\ & \end{bmatrix} \simeq \begin{bmatrix} \left[\underset{\sim}{P}^{K+N_1}_{K+N_1}\right]_{11} & \\ & \bigcirc \end{bmatrix} + \begin{bmatrix} N_2[\underset{\sim}{Q}]_{11} & \\ & \bigcirc \end{bmatrix} + \begin{bmatrix} 0 & \\ & \underset{SS}{\underset{\sim}{Q}} \end{bmatrix}. \tag{5.34}$$

Substituting N_1 for N in (5.21), comparing with (5.34) and using (5.33) leads to

$$\underset{\sim}{P}^{K}_{K+N_1} = \underset{\sim}{P}^{K+N_1}_{K+N_1+N_2}, \qquad N_1 \text{ and } N_2 \text{ sufficiently large.} \quad (5.35)$$

Thus the predicted covariance matrices at each sample time *must be equal.* *The corrected covariance matrices just after both samples may then be* written from (5.3) as follows:

$$\underset{\sim}{P}^{K+N_1}_{K+N_1}\left(\underset{\sim}{C}^{*}_{K+N_1}\right) = \underset{\sim}{P}^{K}_{K+N_1}\left(\underset{\sim}{C}^{*}_{K}\right) - \underset{\sim}{P}^{K}_{K+N_1}\left(\underset{\sim}{C}^{*}_{K}\right)\underset{\sim}{C}^{*T}_{K+N_1}$$

$$\times \left[\underset{\sim}{C}^{*}_{K+N_1}\underset{\sim}{P}^{K}_{K+N_1}\left(\underset{\sim}{C}^{*}_{K}\right)\underset{\sim}{C}^{*T}_{K+N_1} + \underset{\sim}{V}\right]^{-1}\underset{\sim}{C}^{*}_{K+N_1}\underset{\sim}{P}^{K}_{K+N_1}\left(\underset{\sim}{C}^{*}_{K}\right), \quad (5.36A)$$

$$\underset{\sim}{P}^{K+N_1+N_2}_{K+N_1+N_2}\left(\underset{\sim}{C}^{*}_{K+N_1+N_2}\right) = \underset{\sim}{P}^{K+N_1}_{K+N_1+N_2}\left(\underset{\sim}{C}^{*}_{K+N_1}\right) - \underset{\sim}{P}^{K+N_1}_{K+N_1+N_2}\left(\underset{\sim}{C}^{*}_{K+N_1}\right)\underset{\sim}{C}^{*T}_{K+N_1+N_2}$$

$$\times \left[\underset{\sim}{C}^{*}_{K+N_1+N_2}\underset{\sim}{P}^{K+N_1}_{K+N_1+N_2}\left(\underset{\sim}{C}^{*}_{K+N_1}\right)\underset{\sim}{C}^{*T}_{K+N_1+N_2} + \underset{\sim}{V}\right]^{-1}\underset{\sim}{C}^{*}_{K+N_1+N_2}\underset{\sim}{P}^{K+N_1}_{K+N_1+N_2}\left(\underset{\sim}{C}^{*}_{K+N_1}\right). \quad (5.36B)$$

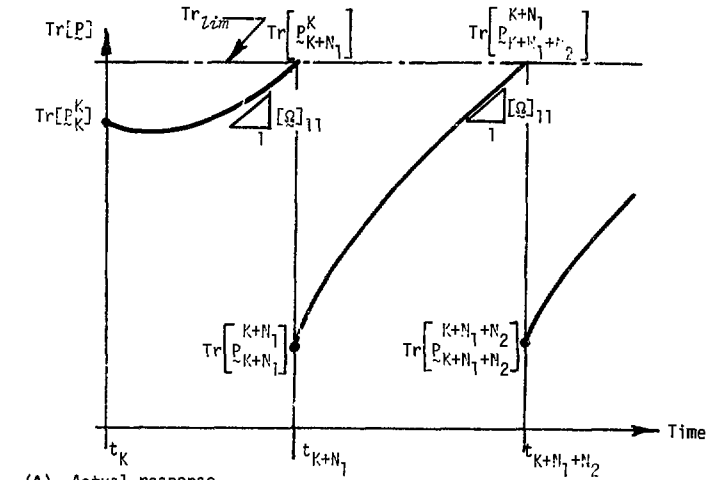
By recognizing that the two predicted covariance matrices are equal from (5.35) equations (5.36) lead to *the* most important result for the monitoring problem:

> Conclusion VI. For the infrequent sampling monitoring problem with a fixed number of samplers and constant error limit, the optimal design of the monitoring system — the optimal number of sensors and their placement — need only be done once, for the same design is optimal for all other measurement times. (C.VI)

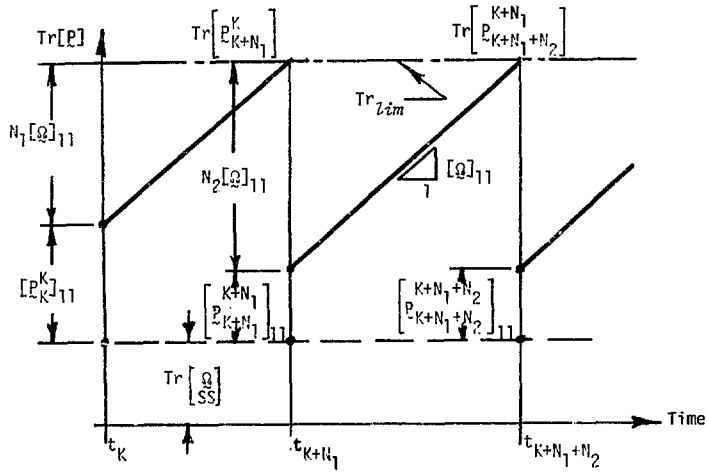
Also, from (5.35) and (5.36) can be seen

> *Conclusion VIA. In the optimal monitoring problem,* measurement times are equally spaced. (C.VIA)

These relationships are illustrated in Figures 5.2A and 5.2B. The first curve represents a typical trajectory of the full trace while the second, the asymptotic approximation. Since $\underset{\sim}{P}^{K}_{K+N_1} = \underset{\sim}{P}^{K}_{K+N_1+N_2}$, the resulting optimal measurement matrices $\underset{\sim}{C}^{*}_{K+N_1}$ and $\underset{\sim}{C}^{*}_{K+N_1+N_2}$ must be the same.



(A) Actual response



(B) Asymptotic approximation

Figure 5.2. The infrequent sampling problem with fixed number of samplers and constant error bound.

5.3.4 Variable Number of Samplers — The case where the number of samplers to be deployed at each measurement time may vary is in general quite difficult. However, in cases where (5.18) applies, the case of infrequent sampling, results can be obtained. If the error limit $Tr_{\mathcal{L}im}$ is constant over the time interval of interest, then the result derives immediately from Conclusion VI:

> Conclusion VII. For the case of infrequent sampling, the optimal number of samplers to use may be found by repetitively solving the optimal design problem for $\underset{\sim}{C}^*_K$ at the first measurement over the range of m=1 to m=n samplers, then extending the results over the full time interval to find which $\underset{\sim}{C}^*_K$ as a function of m leads to the fewest total number of samples. The optimal number of samples to take at each measurement time is the same for all measurement times. (C.VII)

Thus, for infrequent sampling, the optimal number of samplers to use is seen to be constant at each measurement, and that optimal number can be found in a computationally straightforward manner at the first measurement time.

Even though the optimal number of samplers to use at each measurement is a constant, it is important to note that at any specific sample time, the optimal number of samplers to use is independent of the number used in the other samples. This can be seen by comparing (5.31) and (5.32) as was done in (5.33). If m_K samplers had been used at time t_K in the left-hand side of (5.33), m_{K+N_1} could have been used at time t_{K+N_1} in the right-hand side. Since for the case of the equality, the two *sums* in (5.33) must be equal, if the dimension m_K of the measurement on the left-hand side were smaller than m_{K+N_1} on the right-hand side, then in general $\left[\underset{\sim}{P}^K_K\right]_{11}$ would be larger than $\left[\underset{\sim}{P}^{K+N_1}_{K+N_1}\right]_{11}$ and simultaneously N_1 smaller than N_2. Thus, in the case of infrequent sampling, at the sample time t_{K+N_1} in (5.31), the value of the covariance matrix $\underset{\sim}{P}^K_{K+N_1}$ for use in (5.36A) to determine $\underset{\sim}{C}^*_{K+N_1}$ at time t_{K+N_1} is no longer truly a function of $\underset{\sim}{C}^*_K$ nor

of m_K, its dimension. This is so since the sum $\left(\left[P_K^K(C_K^*)\right]_{11} + N[\Omega]_{11}\right)$ in (5.31) is a constant; if C_K^* changes, so will N_1 to maintain the sum at that constant. Thus, since $Tr[\Omega]$ in (5.31) is fixed, and since the other two terms form a constant, the trace $Tr\left[P_{K+N_1}^K\right]$ on the left-hand side is determined *only* by the error limit itself, Tr_{lim}. Hence $P_{K+N_1}^K$ for N_1 large does not directly depend upon C_K^*, even though such a functional relationship is implied by writing $P_{K+N_1}^K(C_K^*)$. Thus, various numbers of samplers could be used at different sample times. However, it is only in considering the solution over the full time interval of interest that the overall optimum is seen to be the use of the same number of samplers at each measurement. This concept is demonstrated at length in the examples in Chapter 6.

5.3.5 Analytical Measurement Optimization — Thus far, the optimal monitoring problem posed in Section 5.2 specialized to the case of bound on error in the state estimate has been found to be equivalent to the minimization of $\left[P_K^K(C_K)\right]_{11}$ as a function of C_K in Conclusion III. Little has been said, however, about the actual determination of C_K^*, the optimal choice of C_K which minimizes the objective function $\left[P_K^K(C_K)\right]_{11}$.

As is well known, analytical methods of obtaining extrema are superior to numerical methods wherever analytical methods exist (see Beveridge and Schechter [20]). Analytical solutions to extremization problems usually exist, however, only for very special cases. A fortunate situation arises in the present case since some work has already been done in dealing with extrema and derivatives of the trace functional (see Athans and Schweppe [11] and Athans [8]).

Pursue an analytical solution of the optimal design problem, which, with the simplifications of Conclusion III, may be stated as follows:

Find the optimal measurement matric $\underset{\sim}{C}_K^*$ such that
$[\underset{\sim}{P}_K^K(\underset{\sim}{C}_K)]_{11}$ is minimized. (5.37)

This is minimization of the first element of the corrected covariance matrix after a sample at time t_K over all choices of possible measurement matrices, $\underset{\sim}{C}_K$. Analytical methods exist for approaching an allied problem which may be stated as follows:

Find the optimal measurement matrix $\underset{\sim}{C}_K^*$ such that
$\mathrm{Tr}[\underset{\sim}{P}_K^K(\underset{\sim}{C}_K)]$ is minimized. (5.38)

As shown in Conclusion II, these are not the same problems. (5.38) is minimizing the trace *at the time of the sample* whereas, by Conclusion II, (5.37) is equivalent to minimizing the trace *for times far beyond the sample* time. However, techniques for the solution of (5.38) could prove to be applicable to (5.37).

Motivated by the computational efficiency of an analytical solution, an attempt is thus made to solve

$$\frac{\partial}{\partial \underset{\sim}{C}_K} \mathrm{Tr}\left[\underset{\sim}{P}_K^K(\underset{\sim}{C}_K)\right] = \underset{\sim}{0}. \tag{5.39}$$

The notation in (5.39) means taking the partial derivative of the trace of $\underset{\sim}{P}_K^K(\underset{\sim}{C}_K)$ (a *scalar*) with respect to $\underset{\sim}{C}_K$ (a *matrix*). This concept has been developed by Athans and Schweppe [11] and applied to a similar problem by Shoemaker [117]. In order to find the stationary matrix solution of (5.39), extensions of concepts of finding extrema in ordinary calculus are made to the case of scalar valued functions of a matrix.

Consider the system starting at time t_0. For a measurement at time t_K, seek $\underset{\sim}{C}_K^*$ such that, using (5.9) in (5.39),

$$\frac{\partial}{\partial \underset{\sim}{C}_K} \mathrm{Tr}\left[\underset{\sim}{P}_K^0 - \underset{\sim}{P}_K^0 \underset{\sim}{C}_K^T \left(\underset{\sim}{C}_K \underset{\sim}{P}_K^0 \underset{\sim}{C}_K^T + \underset{\sim}{V}\right)^{-1} \underset{\sim}{C}_K \underset{\sim}{P}_K^0\right] = \underset{\sim}{0}. \tag{5.40}$$

As detailed in Appendix D, the result is

$$\underset{\sim}{C}_K^* = \underset{\sim}{0}, \tag{5.41}$$

This can be seen to correspond with the case of taking *no* measurements such that the extremum found in (5.40) is actually a *maximum*, not a minimum. An initial attempt was made at constraining the range of $\underset{\sim}{C}_K$ in such minimizations with the method of Lagrange multipliers with no success; more study is still needed of such analytical techniques. One study is currently underway by Shoemaker [117] in which restricted classes of problems are treated through the use of analytical techniques; such methods were not found to be appropriate for use in this study since they require n measurements at each sample time, a severe restriction.

Alternate performance indices to that used in (5.40) yield matrix equations whose solutions are not known, so that the analytical approach with the trace function is not found to be fruitful; see Appendix D.

It can be shown that attempting to solve the more germane problem of finding $\underset{\sim}{C}_K^*$ in (5.37) such that

$$\frac{\partial}{\partial \underset{\sim}{C}_K}\left[\underset{\sim}{P}_K^K(\underset{\sim}{C}_K)\right]_{11} = \underset{\sim}{0} \tag{5.42}$$

also results in sets of equations for which solutions are not known. An even more appropriate optimization problem might be to maximize the time itself between required measurements. For the discrete-time formulation used here, however, this is equivalent to finding

$$\frac{\partial}{\partial \underset{\sim}{C}_K} N = \underset{\sim}{0},$$

where N is the number of timesteps between samples. Solutions to this problem were pursued but led to less conclusive results since, due to the discrete nature of N, many choices of $\underset{\sim}{C}_K$ resulted in the same maximum value for N. Thus, the analytical approach, though instructive in

the area of matrix calculus, is abandoned as a means of solving the monitoring problem (see Appendix D for details of gradient matrices for the trace function and its calculus).

5.3.6 Numerical Measurement Position Optimization — In the last section, attempts were made at analytical minimization of $\mathrm{Tr}\left[\underset{\sim}{P}_K^K(\underset{\sim}{C}_K)\right]$ or $\left[\underset{\sim}{P}_K^K(\underset{\sim}{C}_K)\right]_{11}$ with respect to the matrix $\underset{\sim}{C}_K$ itself. A fundamental question underlies extremization of measurement functionals directly with respect to the elements of the measurement matric $\underset{\sim}{C}_K$; once $\underset{\sim}{C}_K$ is found, how is it related to the vector of actual optimal sensor locations in the medium, $\underset{\sim}{z}_K^*$? None of the studies of measurement system optimization found in the literature adequately addresses the optimal measurement design problem from the point of view of optimal *placement* determination.

The normal-mode formulation of the diffusion problem is introduced as a means of tying together $\underset{\sim}{C}_K$ and $\underset{\sim}{z}_K$. For the case of one-dimensional diffusion with the no-flow condition at the boundaries, from (3.39), write $\underset{\sim}{C}_K$ as a function of $\underset{\sim}{z}_K$ as follows:

$$\underset{\sim}{C}(\underset{\sim}{z}_K) \equiv \begin{bmatrix} 1 & \cos\left(\frac{\pi}{2L} z_1\right) & \cos\left(2\frac{\pi}{2L} z_1\right) \cdots & \cos\left((n-1)\frac{\pi}{2L} z_1\right) \\ 1 & \cos\left(\frac{\pi}{2L} z_2\right) & \cos\left(2\frac{\pi}{2L} z_2\right) \cdots & \cos\left((n-1)\frac{\pi}{2L} z_2\right) \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ 1 & \cos\left(\frac{\pi}{2L} z_m\right) & & \end{bmatrix} \quad (5.43)$$

Thus, $\underset{\sim}{C}_K$ is a continuous function of $\underset{\sim}{z}_K$ so that all the conclusions developed thus far apply with $\underset{\sim}{C}(\underset{\sim}{z}_K)$ substituted for $\underset{\sim}{C}_K$ and for minimization with respect to $\underset{\sim}{z}_K$ instead of $\underset{\sim}{C}_K$.

For example, with the use of $\underset{\sim}{C}(\underset{\sim}{z}_K)$ as defined in (5.43), Conclusion III may be written as follows:

Conclusion IIIA. For N large, to maximize t_{K+N}, the time when $\mathrm{Tr}[\underset{\sim}{P}_{K+N}(\underset{\sim}{C}(z_K))] > \mathrm{Tr}\,\underset{\sim}{P}_{lim}$, choose that z_K at time t_K which minimizes $[\underset{\sim}{P}_K(\underset{\sim}{C}(z_K))]_{11}$. (C.IIIA)

Consider the problem of the minimization of the scalar-valued objective function $\left[\underset{\sim}{P}_K\left(\underset{\sim}{C}(z_K)\right)\right]_{11}$ of a vector z_K. Such problems have received considerable attention. (An adequate coverage of the various techniques may be found in Beveridge and Schechter [20].) The monitoring problem, where the allowable positions of the samplers are constrained to lie somewhere within the region of the medium, suggests consideration of constrained optimization techniques. There are various types of constrained minimization methods, methods requiring use of only the objective function itself (so called direct methods), methods which require the objective function and its gradient (first-order gradient methods) and those which in addition require the Hessian of the objective function (second-order gradient methods). Second-order gradient methods are often the fastest of available methods [103]. Thus, in the interest of numerical efficiency, such second-order methods are considered.

Define the objective function of interest to correspond with Conclusion IIIA:

$$J(z_K) \equiv \left[\underset{\sim}{P}_K^0 - \underset{\sim}{P}_K^0\underset{\sim}{C}^T(z_K)\left\{\underset{\sim}{C}(z_K)\underset{\sim}{P}_K^0\underset{\sim}{C}^T(z_K) + \underset{\sim}{V}\right\}^{-1}\underset{\sim}{C}(z_K)\underset{\sim}{P}_K^0\right]_{11}. \tag{5.44}$$

As shown by Athans and Schweppe [11] for the case of the trace operator *Tr[·], the total differential and trace operators are linear so that* (see Appendix D)

$$d\mathrm{Tr}[\underset{\sim}{X}] = \mathrm{Tr}[d\underset{\sim}{X}]. \tag{5.45}$$

Similarly, in (5.44), what may be called the "$[\cdot]_{11}$-operator" is also linear, being a linear part of the trace, so that

$$d[\underset{\sim}{X}]_{11} = [d\underset{\sim}{X}]_{11}. \tag{5.46}$$

From Appendix D,

$$d\underline{X}^{-1} = -\underline{X}^{-1}(d\underline{X})\underline{X}^{-1}. \tag{5.47}$$

Define

$$\underline{T} \equiv \left\{\underline{C}(\underline{z}_K)\underline{P}_K^0\underline{C}^T(\underline{z}_K) + \underline{V}\right\}. \tag{5.48}$$

(5.46), (5.47), and (5.48) are used with (5.44) to find the gradient of the objective function which may be written as follows:

$$\frac{\partial}{\partial \underline{z}_K} J(\underline{z}_K) = -\sum_{i=1}^{m} \underline{e}_i \left[\underline{P}_K^0\left(\frac{\partial}{\partial z_i}\underline{C}(\underline{z}_K)^T\right)\underline{T}^{-1}\underline{C}(\underline{z}_K)\underline{P}_K^0 - \underline{P}_K^0\underline{C}(\underline{z}_K)^T\underline{T}^{-1}\left\{\left(\frac{\partial}{\partial z_i}\underline{C}(\underline{z}_K)\right)\underline{P}_K^0\underline{C}(\underline{z}_K)^T + \underline{C}(\underline{z}_K)\underline{P}_K^0\left(\frac{\partial}{\partial z_i}\underline{C}(\underline{z}_K)^T\right)\right\}\underline{T}^{-1}\underline{C}(\underline{z}_K)\underline{P}_K^0 + \underline{P}_K^0\underline{C}(\underline{z}_K)^T\underline{T}^{-1}\left(\frac{\partial}{\partial z_i}\underline{C}(\underline{z}_K)\right)\underline{P}_K^0\right]_{11}, \tag{5.49}$$

where the unit vector $\underline{e}_i \equiv [0,0,1,0,\ldots,0]^T$, the 1 in the ith element. Thus, the gradient of $J(\underline{z}_K)$ may be written analytically in a straightforward manner. Note that the inverse $\underline{T}^{-1}$ need be computed only once per evaluation of the gradient and that it is an $(m \times m)$ matrix, not an $(n \times n)$ matrix. Usually, the number of measurement sensors m is smaller than the number of states in the model n so that this inversion is computationally manageable. (As a historical note, this quality of inverting the smaller $(m \times m)$ matrix was one of the important features inherent in the practical utility of the Kalman Filter; see Jazwinski [65].)

For the second-order gradient of $J(\underline{z}_K)$, known as the Hessian, adopt for the time being the following notation:

(1) Drop the time subscript K, the tildas, and the functional relationship so that $C \equiv \underline{C}(\underline{z}_K)$, $P \equiv \underline{P}_K^0$;

(2) $C_i \equiv \frac{\partial}{\partial z_i}\underline{C}(\underline{z}_K)$;

(3) $C_{ij} \equiv \frac{\partial^2}{\partial z_i \partial z_j}\underline{C}(\underline{z}_K)$. (5.50)

With (5.50), differentiate the ith element of (5.49) with respect to the jth element of z_K to obtain the (i,j)th element of the Hessian as follows:

$$\begin{aligned}
\frac{\partial^2}{\partial z_i \partial z_j} J = -\Big[& P\left(C_{ij}^T\right)T^{-1}CP - P\left(C_j^T\right)T^{-1}\left\{\left(C_i^T\right)PC^T + CP\left(C_i^T\right)\right\}T^{-1}CP \\
& + P\left(C_j^T\right)T^{-1}\left(C_i\right)P + P\left(C_i^T\right)T^{-1}\left(C_j\right)P \\
& - PC^TT^{-1}\left\{\left(C_i\right)PC^T + CP\left(C_i^T\right)\right\}T^{-1}\left(C_j\right)P \\
& + PC^T\,T^{-1}\left(C_{ij}\right)P - P\left(C_i^T\right)T^{-1}\left(C_j\right)PC^TT^{-1}CP \\
& + PC^TT^{-1}\left\{\left(C_i\right)PC^T + CP\left(C_i^T\right)\right\}T^{-1}\left(C_j\right)PC^TT^{-1}CP \\
& - PC^TT^{-1}\left(C_{ij}\right)PC^TT^{-1}CP - PC^TT^{-1}\left(C_j\right)P\left(C_i^T\right)T^{-1}CP \\
& + PC^TT^{-1}\left(C_j\right)PC^TT^{-1}\left\{\left(C_i\right)PC^T + CP\left(C_i^T\right)\right\}T^{-1}CP \\
& - PC^TT^{-1}\left(C_j\right)PC^TT^{-1}\left(C_i\right)P - P\left(C_i^T\right)T^{-1}CP\left(C_j^T\right)T^{-1}CP \\
& + PC^TT^{-1}\left\{\left(C_i\right)PC^T + CP\left(C_i^T\right)\right\}T^{-1}CP\left(C_j^T\right)T^{-1}CP \\
& - PC^TT^{-1}\left(C_i\right)P\left(C_j^T\right)T^{-1}CP - PC^TT^{-1}CP\left(C_{ij}^T\right)T^{-1}CP \\
& + PC^TT^{-1}CP\left(C_j^T\right)T^{-1}\left\{\left(C_i\right)PC^T + CP\left(C_i^T\right)\right\}T^{-1}CP \\
& - PC^TT^{-1}CP\left(C_j^T\right)T^{-1}\left(C_i\right)P\Big]_{11}
\end{aligned} \tag{5.51}$$

This represents *only one term* of the $m \times m$ Hessian matrix which would be given by

$$\frac{\partial^2}{\partial \underset{\sim}{z}_K^2} J(\underset{\sim}{z}_K) = \sum_{i=1}^{m}\sum_{j=1}^{m} \underset{\sim}{E}_{ij} \frac{\partial^2}{\partial z_i \partial z_j} J, \tag{5.52}$$

where $\underset{\sim}{E}_{ij}$ is a unit matrix.

The computational efficiency of second-order gradient methods is seen to be lost in the horrendous task of defining the Hessian of the objective function and for that reason, *first-order* gradient methods are sought.

Before going on to first-order gradient methods, a word about direct search methods is in order. While in general less efficient than gradient techniques, direct search methods possess the distinction of not requiring an analytical expression for the gradient, an important practical advantage. This is of significance first since it permits a user to proceed much more rapidly from his problem statement to its coded form for numerical solution. Secondly, and more importantly, the vast majority of physical problems do not admit the writing of an analytical expression for the gradient so that for those problems, direct search methods are all that is available. An interesting example of a direct search technique is that due to Radcliffe and Comfort [103] in which Powell's unconstrained conjugate directions minimization procedure without derivatives [103] is extended to the case including nonlinear equality and inequality constraints. However, in the monitoring problem, it is a straightforward process to define a gradient of the form (5.49) so that first-order gradient methods are preferred over direct methods for their computational efficiency.

The algorithm chosen for finding the minimum of $J(\underline{z}_K)$ in (5.44) was written by G. W. Westley and is named KEELE [127]. It is an algorithm to find a *local* minimum of a function of many variables where the variables are subject to linear inequality and/or linear equality constraints. It represents an extension of a Davidon variable metric procedure reported by Fletcher and Powell [127] using gradient projection methods (see Rosen [54]) to include the case of linear constraints.

Note how in the monitoring problem, it is necessary to constrain the ranges of the variables so that resultant monitoring positions bear physical significance to the problem statement. Note also how only linear,

not nonlinear, constraints are required: each of the elements of $\underset{\sim}{z}_K^*$ must satisfy a constraint of the form

$$0 \leq z_i^* \leq 2L, \qquad i = 1,2,\ldots,m, \tag{5.53}$$

where the one-dimensional medium is of length 2L.

Note how this algorithm, and all gradient algorithms, seek only local, not global, minima. The only way known to approach solution of the global minimization problem is by solving a sequence of local minimization problems starting from different initial guesses until some measure indicates probable convergence to the global minimum (see Beveridge and Schechter [20], p. 499 and Radcliffe and Comfort [103], p. 3). For this reason KEELE has been modified to include random initialization of the starting vector $\underset{\sim}{z}_K$. This technique has been found to yield satisfactory results provided a sufficient number of random starting points is used in each attempt at finding a global minimum in $J(\underset{\sim}{z}_K)$.

Thus, within the probability that the best local minimum found is the global minimum, the optimal positioning of the m samplers at any time t_K is considered solved.

5.3.7 Numerical Measurement Quality Optimization — The last question left to answer at a measurement time in the design problem of Section 5.1 is what *types* of sensors to deploy at a sample? Consider the filter equations of relevance for a measurement at time t_K:

$$\underset{\sim}{y}_K = \underset{\sim}{C}(\underset{\sim}{z}_K)\underset{\sim}{x}_K + \underset{\sim}{v}_K, \tag{5.54}$$

$$\underset{\sim}{P}_K^K = \underset{\sim}{P}_K^O - \underset{\sim}{P}_K^O\underset{\sim}{C}(\underset{\sim}{z}_K)^T\left[\underset{\sim}{C}(\underset{\sim}{z}_K)\ \underset{\sim}{P}_K^O\underset{\sim}{C}(\underset{\sim}{z}_K)^T + \underset{\sim}{V}\right]^{-1}\underset{\sim}{C}(\underset{\sim}{z}_K)\underset{\sim}{P}_K^O, \tag{5.55}$$

$$\underline{G}_K = \underline{P}_K^0 \underline{C}(\underline{z}_K)^T \left[\underline{C}(\underline{z}_K)\ \underline{P}_K^0 \underline{C}(\underline{z}_K)^T + \underline{V} \right]^{-1}, \tag{5.56}$$

$$\hat{\underline{x}}_K^K = \hat{\underline{x}}_K^0 + \underline{G}_K \left[\underline{y}_K - \underline{C}(\underline{z}_K) \hat{\underline{x}}_K^0 \right]. \tag{5.57}$$

As presented in Chapter 4, the noise-corrupted measurements in (5.54) are characterized by mean vector and covariance matrix given as follows:

$$E\left[\underline{v}_K\right] \equiv \underline{0},$$

$$E\left[\underline{v}_K \underline{v}_J^T\right] \equiv \underline{V} \delta_{KJ}. \tag{4.18}$$

Thus, the additive measurement noise forms a sequence of zero-mean, white, Gaussian random vectors with covariance given by $\underline{V}$. To conform to this problem structure, the only variables left to determine in specifying the sensors at a measurement are the strengths of the noise terms in $\underline{v}_K$ as defined by their covariances, the elements $[\underline{V}]_{ij}$ of the covariance matrix $\underline{V}$. From the theory of random variables, if the measurements in (5.54) are made with *independent* sensors, the elements of $\underline{v}_K$, the individual random errors among the samples taken, will be uncorrelated. For this case, $\underline{V}$ is a diagonal matrix which leaves only the specification of the m elements $[\underline{V}]_{ii}$, $i = 1,2,\ldots,m$. The diagonal elements of $\underline{V}$ may be interpreted as the mean-square values of the errors in each of the m samples. Thus, their sizes are inversely related to the quality of the measurement instrument used so that if a high quality sample is desired for $[\underline{y}_K]_i$, then $[\underline{V}]_{ii}$ should be small, and vice versa.

Thus, if the sole objective in the solution of the monitoring problem is to minimize the total *number* of samples necessary over the entire time interval, the optimal choice of measurement instruments is clearly that choice which leads to the most accurate measurement — use the highest accuracy sensor available. If, on the other hand, the more meaningful

measure of minimizing the total monitoring program *cost* is to be used in the overall optimization, a more complicated problem structure results. Contributions to the total cost could include costs associated with every sample that is taken, a quantized cost range associated with available measurement instruments of various accuracies, etc. Tradeoffs result between taking a large number of low accuracy measurements and a small number of high accuracy measurements at a sample time.

Though this aspect of the total problem is an important part of the complete optimal design, it is left for later study with an outline of the structure of its inclusion within the infrequent sampling problem framework given in Appendix E.

What is clear from the conclusions so far, is that once the optimal choice of measurement instruments is made for one sample, that choice is optimal for all other samples which leads to the final result for the monitoring design problem with bound on error in the state estimate:

> Conclusion VIII. For the case of infrequent sampling, the complete solution of the optimal monitoring design problem with constant bound on error in the state estimate — the determination of the optimal number of samplers to use at each measurement, their optimal locations and the optimal choice of measurement instrument accuracies — may be obtained at the first measurement time, with the same design being optimal for all other measurement times. (C.VIII)

5.4 The Design Problem for a Bound on the Error in the Output Estimate

5.4.1 *The Minimax Problem* — The second form of the monitoring design problem is considered in this section. It is required to make the fewest measurements possible over the time interval of interest while maintaining the error in the estimate of the pollutant concentration itself, the output, within some bound everywhere in the medium. This is a

more complex situation than that of maintaining the error in the state within some bound; the pollutant concentration over the whole region must lie within the error constraint so that the entire region must be considered when testing for violation of the constraint.

At time t_K, let the pollutant concentration at a point z in a one-dimensional diffusive medium of length 2L be given by

$$\xi_K(z) \equiv \underline{c}(z)^T \underline{x}_K, \tag{5.58}$$

where the *vector* $\underline{c}(z)^T$ for the *scalar output* $\xi_K(z)$ is much like the measurement *matrix* $\underline{C}(z_K)$ for the *vector measurement* $\underline{y}_K$ in (5.43) and is given by

$$\underline{c}(z)^T = \left[1, \cos\left(\frac{\pi}{2L} z\right), \cos\left(2\frac{\pi}{2L} z\right), \ldots, \cos\left((n-1)\frac{\pi}{2L} z\right)\right]. \tag{5.59}$$

Equations (5.58) and (5.59) are formalizations of the series expression in (3.41) and can be seen schematically in the bond graph in Figure 3.2. The pollutant concentration at any point is thus simply the sum of the modal concentrations at that point in the medium.

Equation (5.58) applies for the *estimated* pollutant concentration from the filter as well and may be written as

$$\hat{\xi}_K(z) \equiv \underline{c}(z)^T \hat{\underline{x}}_K^0, \tag{5.60}$$

where $\hat{\underline{x}}_K^0$ is the value of the state estimate predicted to time t_K from time t_0 (see (C.18) in Appendix C). It is required to maintain the error in this estimate to be within some bound. Since $\xi_K(z)$ is a scalar random variable, an expression of the error between the estimate $\hat{\xi}_K(z)$ and the actual value $\xi_K(z)$ in the mean-square sense is the variance in the estimate. The variance in the estimate of the output in (5.60) is found to be

$$\sigma_K^2(z) \equiv E\left[\left(\hat{\xi}_K(z) - \xi_K(z)\right)^2\right]$$

$$= E\left[\left(\underset{\sim}{c}(z)^T\left\{\hat{\underset{\sim}{x}}_K^0 - \underset{\sim}{x}_K\right\}\right)\left(\underset{\sim}{c}(z)^T\left\{\hat{\underset{\sim}{x}}_K^0 - \underset{\sim}{x}_K\right\}\right)^T\right]$$

$$= E\left[\underset{\sim}{c}(z)^T\left\{\hat{\underset{\sim}{x}}_K^0 - \underset{\sim}{x}_K\right\}\left\{\hat{\underset{\sim}{x}}_K^0 - \underset{\sim}{x}_K\right\}^T\underset{\sim}{c}(z)\right]$$

$$= \underset{\sim}{c}(z)^T E\left[\left(\hat{\underset{\sim}{x}}_K^0 - \underset{\sim}{x}_K\right)\left(\hat{\underset{\sim}{x}}_K^0 - \underset{\sim}{x}_K\right)^T\right]\underset{\sim}{c}(z)$$

$$\equiv \underset{\sim}{c}(z)^T\underset{\sim}{P}_K^0\underset{\sim}{c}(z) \qquad (5.61)$$

where the last line follows from the definition of the predicted covariance matrix, equation (4.21). Thus, at time t_K, associated with the *estimate* of the pollutant concentration at any point z given by $\hat{\xi}_K(z)$ is its variance $\sigma_K^2(z)$, a measure of the error in that estimate, which is merely a function of the predicted state estimate error covariance matrix, whose properties are by now well established.

Since the monitoring problem with a bound on the error in the output stipulates that *everywhere* in the medium, at all times over the time interval of interest, the fewest number of measurements must be made to keep the error in the output below a limit, the concern is with checking the *maximum* value of the variance $\sigma_K^2(z)$ for all z over the length of the medium as time goes on to find when the error limit is reached. The assumption is, as it was for the problem with bound on error in the state estimate, that at the time when the error in the estimate of the output reaches its limit, a measurement should be made. That measurement should be made so that the time before the error limit is next reached is maximized; extension of the local optimal design for one measurement period to the overall time interval is assumed possible, the proof of which will be considered later in Section 5.8 dealing with the optimal management problem.

Suppose at time t_K, the variance in the estimate of the output at some point z in the medium is in violation of the error limit defined as σ^2_{lim}, that is,

$$\sigma^2_K(z) \geq \sigma^2_{lim}. \tag{5.62}$$

It is required to make a measurement at time t_K that will result in the longest possible time, say t_{K+N}, when the error limit is reached again. This will occur when, at some point z in the medium, the maximum value of the variance over all other locations in the medium exceeds the limit. This suggests the following algorithm for finding the optimal measurement design at time t_K that will result in the longest time t_{K+N} when another measurement is necessary:

1) Select, in some manner, a measurement design at time t_K and make a measurement;
2) Predict ahead to time t_{K+1};
3) Find the position z^* of the maximum variance
$$\max_z \sigma^2_{K+1}(z);$$
4) Test for violation of the error limit
$$\max_z \sigma^2_{K+1}(z) \geq \sigma^2_{lim};$$
5) If violated, go to (6);
If not violated, increment time one step and return to (2);
6) Store the time when the limit was violated in N_i;
7) Check for convergence to the global maximum t_{K+N^*}
If not satisfied, return to (1), reinitialize time to t_K and select a different trial measurement;
If convergence has occurred, the optimal design is that which resulted in largest N_i, the longest time t_{K+N_i}, call it t_{K+N^*}. (5.63)

Such a direct search technique would be costly to implement. The efficiencies of gradient techniques do not apply since a gradient of the objective function (which would literally be N_i, the time to the next measurement) with respect to the measurement design variables cannot be

expressed analytically. Thus, more information is sought from the structure of the problem to avoid using direct search methods.

As in Section 5.3.7, exclude for now the choice of measurement instrument accuracy from the monitoring design problem. Consider only the choice of the *number* of samplers m to be used in the measurement at time t_K and their optimal *locations*, which are the elements of the m-vector $\underline{z}_K$. Then, the algorithm (5.63) may be concisely written as a minimax problem as follows:

$$\text{Find } \min_{\underline{z}_K} \max_{z} \sigma^2_{K+N}(\underline{z}_K, z) \geq \sigma^2_{lim}. \tag{5.64}$$

In general, such a minimax problem is quite difficult, requiring advanced techniques of mathematical programming for its solution. However, in the case of infrequent sampling, the solution of (5.64) is virtually complete in the earlier results of this chapter.

In order to solve (5.64), from the definition of $\sigma^2_K(z)$ in (5.61), obtain the following:

$$\sigma^2_{K+N}(\underline{z}_K, z) \equiv \underline{c}(z)^T \underline{P}^K_{K+N}(\underline{z}_K)\underline{c}(z) = \underline{c}(z)^T \left[\underline{\Phi}^N \underline{P}^K_K(\underline{z}_K) \underline{\Phi}^{N^T} + \sum_{n=1}^{N} \underline{\Phi}^{n-1} \underline{\Omega} \underline{\Phi}^{n-1^T} \right] \underline{c}(z), \tag{5.65}$$

where

$$\underline{P}^K_K(\underline{z}_K) = \underline{P}^0_K - \underline{P}^0_K \underline{c}(\underline{z}_K)^T \left[\underline{c}(\underline{z}_K) \underline{P}^0_K \underline{c}(\underline{z}_K)^T + \underline{v} \right]^{-1} \underline{c}(\underline{z}_K) \underline{P}^0_K \tag{5.66}$$

is the corrected error covariance matrix just after the first measurement at time t_K, as a function of $\underline{c}(\cdot)$ of $\underline{z}_K$ in (5.43). Expand (5.65):

$$\sigma^2_{K+N}(\underline{z}_K, z) = \underline{c}(z)^T \underline{\Phi}^N \underline{P}^K_K(\underline{z}_K) \underline{\Phi}^{N^T} \underline{c}(z) + \underline{c}(z)^T \sum_{n=1}^{N} \underline{\Phi}^{n-1} \underline{\Omega} \underline{\Phi}^{n-1^T} \underline{c}(z), \tag{5.67}$$

to find the same combination of zero-input response and zero-state response that was found in equation (5.10).

For the physically interesting case of no-flow boundary conditions in one-dimensional diffusion, the eigenvalues of $\underline{A}$ in the state equation (4.1) lead to the ordering of the terms in $\underline{\Phi}$ given by property (5.16). For N sufficiently large, conditions (5.18) and (5.20) are satisfied so that (5.67) may be written as matrices to show

$$\sigma^2_{K+N}(\underline{z}_K,z) \doteq \left[1 \quad \cos\left(\tfrac{\pi}{2L}z\right) \quad \cdots\right] \begin{bmatrix} \left[\underline{P}^K_K(\underline{z}_K)\right]_{11} & & \\ & \bigcirc & \\ & & \underline{\Omega}_{SS} \end{bmatrix} \begin{bmatrix} 1 \\ \cos\left(\tfrac{\pi}{2L}z\right) \\ \cdot \\ \cdot \\ \cdot \end{bmatrix}$$

$$+ \left[1 \quad \cos\left(\tfrac{\pi}{2L}z\right) \quad \cdots\right] \begin{bmatrix} N[\Omega]_{11} & & \\ & \bigcirc & \\ & & 0 \end{bmatrix} \begin{bmatrix} 1 \\ \cos\left(\tfrac{\pi}{2L}z\right) \\ \cdot \\ \cdot \\ \cdot \end{bmatrix}$$

$$+ \left[1 \quad \cos\left(\tfrac{\pi}{2L}z\right) \quad \cdots\right] \begin{bmatrix} 0 & & \\ & \bigcirc & \\ & & \underline{\Omega}_{SS} \end{bmatrix} \begin{bmatrix} 1 \\ \cos\left(\tfrac{\pi}{2L}z\right) \\ \cdot \\ \cdot \\ \cdot \end{bmatrix} \qquad (5.68)$$

from which *the most* important result for the monitoring problem with bound on output error derives; for N sufficiently large,

$$\sigma^2_{K+N}(\underline{z}_K,z) \doteq \left[\underline{P}^K_K(\underline{z}_K)\right]_{11} + N[\Omega]_{11} + \underline{c}(z)^T \underline{\Omega}_{SS} \underline{c}(z). \qquad (5.69)$$

Notice that in the asymptotic case for N sufficiently large, even though σ^2_{K+N} at time t_{K+N} is a function of both $\underline{z}_K$, the positions of the measurement devices at time t_K, and z, the location in the medium where the variance is being tested at time t_{K+N}, the functional relationship *separates*

into independent functions of each argument. The selection of measurement positions $\underset{\sim}{z}_K$ is seen to effect only $\left[\underset{\sim}{P}_K^K(\underset{\sim}{z}_K)\right]_{11}$, exactly as it did in the problem with bound on state error (see equation (5.22)). The location z in the medium where σ^2_{K+N} is being tested effects only the variance associated with the steady-state term of the matrix convolution of the input disturbance statistics, where the matrix $\underset{\sim}{\Omega}_{SS}$ was defined in (5.20) and (5.21). The second term on the right-hand side of (5.69), $N[\underset{\sim}{\Omega}]_{11}$, represents the increase in uncertainty in the estimate of the first mode, which has a constant value throughout the medium, and thus is a function of neither $\underset{\sim}{z}_K$ nor z.

This may be summarized as follows:

> Conclusion IX. For infrequent sampling, the variance in the estimate of the pollutant concentration, the output of the monitor at time t_{K+N}, separates into independent functions of the measurement positions at time t_K and of the pollutant concentration position at time t_{K+N}. (C.IX)

Returning to the minimax problem stated in (5.64), application of Conclusion IX leads to the following fortuitous result:

> Conclusion X. For infrequent sampling the following problems are equivalent:
> (1) Find $\underset{\sim}{z}_K^*$ at time t_K and z^* at time t_{K+N} such that
>
> $$\min_{\underset{\sim}{z}_K} \max_{z} \sigma^2_{K+N}\left(\underset{\sim}{z}_K, z\right) \geq \sigma^2_{lim};$$
>
> (2) Find $\underset{\sim}{z}_K^*$ at time t_K and z^* at time t_{K+N} such that
>
> $$\min_{\underset{\sim}{z}_K} \left[\underset{\sim}{P}_K^K(\underset{\sim}{z}_K)\right]_{11} + N[\underset{\sim}{\Omega}]_{11} + \max_{z} \underset{\sim}{c}(z)^T \underset{SS}{\underset{\sim}{\Omega}} \underset{\sim}{c}(z) \geq \sigma^2_{lim}. \quad (C.X)$$

This result reduces the solution of the monitoring design problem from the completely unmanageable task of (5.63) to the relatively simple combination of two separate problems in minimization and maximization. Solution of the former is identical to that treated in the monitoring problem with bound on error in the state estimate as detailed in the section on

numerical measurement position optimization, Section 5.3.6. Finding $\underset{\sim}{z}_K^*$ at time t_K such that $\left[P_K^K(z_K)\right]_{11}$ is minimized results in the smallest contribution due to the initial covariance at time t_K to the variance in the output at time t_{K+N}.

Solution of the latter problem, the maximization of the variance due to the steady-state convolution matrix at time t_{K+N} is developed in the following. From (5.17) and (5.21), an expression for the variance associated with the zero-state, or forced, response in (5.67) may be expanded as matrices as follows:

$$\underset{\sim}{c}(z)^T \sum_{n=1}^{N} \underset{\sim}{\Phi}^{n-1} \underset{\sim}{\Omega} \underset{\sim}{\Phi}^{n-1T} \underset{\sim}{c}(z) \equiv \underset{\sim}{c}(z)^T \underset{N}{\underset{\sim}{\Omega}} \underset{\sim}{c}(z) =$$

$$\left[1 \quad \cos\left(\frac{\pi}{2L} z\right) \quad \cdots\right] \begin{bmatrix} N[\Omega]_{11} & [\Omega]_{12} \sum_{n=1}^{N} \phi_{11}^{n-1} \phi_{22}^{n-1} & \cdots \\ [\Omega]_{21} \sum_{n=1}^{N} \phi_{22}^{n-1} \phi_{11}^{n-1} & [\Omega]_{22} \sum_{n=1}^{N} \phi_{22}^{2(n-1)} & \\ \vdots & & \end{bmatrix} \begin{bmatrix} 1 \\ \cos\left(\frac{\pi}{2L} z\right) \\ \vdots \end{bmatrix} \tag{5.70}$$

As before,

$$\lim_{N \to \infty} [\Omega]_{ij} \sum_{n=1}^{N} \phi_{ii}^{n-1} \phi_{jj}^{n-1} = \underset{SS}{[\Omega]}_{ij}, \tag{5.20}$$

so that every element of the matrix convolution in (5.70) approaches its steady-state value as N becomes large *except the first*, which grows as a ramp with slope $[\Omega]_{11}$. Thus, for N large,

$$\underset{\sim}{c}(z)^T \sum_{n=1}^{N} \underset{\sim}{\Phi}^{n-1} \underset{\sim}{\Omega} \underset{\sim}{\Phi}^{n-1T} \underset{\sim}{c}(z) \doteq N[\Omega]_{11} + \underset{\sim}{c}(z)^T \underset{SS}{\underset{\sim}{\Omega}} \underset{\sim}{c}(z). \tag{5.71}$$

It is to be emphasized that as the limit in (5.20) is approached, the variance associated with the matrix convolution (5.71) separates into a time-varying term and a term which is a *constant*. Thus, for N sufficiently large, the only term involving z in the expression for $\sigma^2_{K+N}(\underset{\sim}{z}_K,z)$ is *not a function of time* and can be precalculated independently of the actual time that the error limit σ^2_{lim} is reached in (5.64). This separates determinization of the maximum over z of $\sigma^2_{K+N}(\underset{\sim}{z}_K,z)$ from the actual value of N, and thus t_{K+N}, provided only that N is sufficiently large for (5.20) to apply.

The relationships in Conclusion X are portrayed graphically in Figure 5.3A and B. Figure 5.3A depicts the actual evolution of σ^2 with time whereas 5.3B shows the asymptotic relationships of (5.69). The important point is that the last term in (5.69), the term involving z, has the *same maximum* as a function of z *at each sample* so long as the number of time steps between each pair of samples is sufficiently large. Thus,

> Conclusion XI. The position of the maximum variance in the estimate of pollutant concentration at the time each measurement is required in the monitoring problem with bound on error in the output is independent of time, provided the time between measurements is sufficiently large, and is thus the same position at every measurement. (C.XI)

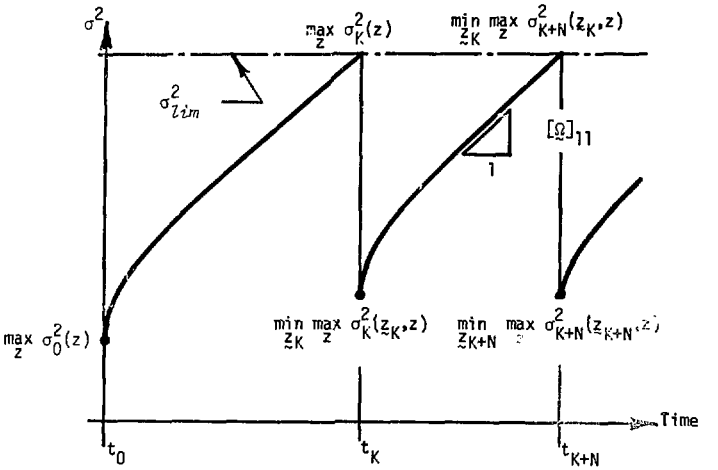
The procedure for the solution of the infrequent monitoring problem with bound on error in the output estimate is as follows:

(1) At time t_K, solve for the optimal measurement positions $\underset{\sim}{z}^*_K$ such that

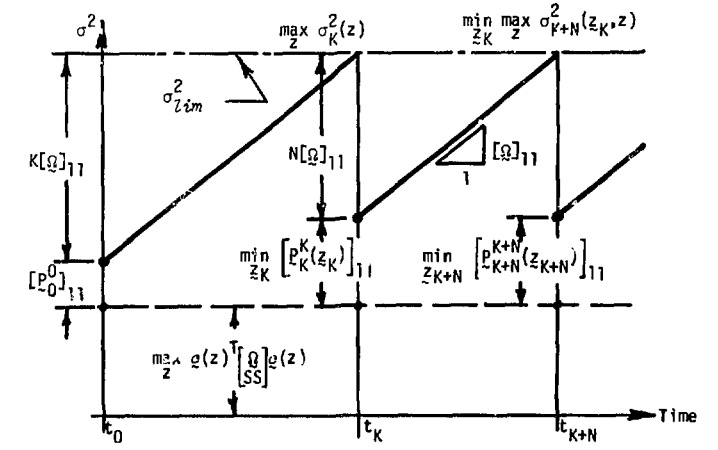
$$P^*_{11} = \min_{\underset{\sim}{z}_K} \left[\underset{\sim}{P}^K_K(\underset{\sim}{z}_K)\right]_{11};$$

(2) Compute $\left[\underset{\sim}{\Omega}_{SS}\right]$ using the relationships

$$\left[\underset{\sim}{\Omega}_{SS}\right]_{ij} = \frac{[\Omega]_{ij}}{1 - \phi_{ii}\phi_{jj}}, \quad i \text{ and } j \neq 1, \quad \left[\underset{\sim}{\Omega}_{SS}\right]_{11} = 0;$$



(A) Actual response



(B) Asymptotic approximation

Figure 5.3. The infrequent sampling problem with bound on error in the output estimate.

(3) Find N large enough that the infrequent sampling approximations apply, that is, so that

$$\left[\underset{\sim}{\Omega}_{N}\right]_{ij} \equiv [\underset{\sim}{\Omega}]_{ij} \sum_{n=1}^{N} \phi_{ii}^{n-1} \phi_{jj}^{n-1} \simeq \left[\underset{\sim}{\Omega}_{SS}\right]_{ij}, \quad i \text{ and } j \neq 1;$$

(4) Find z^*, the position where the variance approaches its steady-state maximum, where
$\sigma^2_{SS} = \max_{z} \underset{\sim}{c}(z)^T \underset{\sim}{\Omega}_{SS} \underset{\sim}{c}(z)$;

(5) For the pair (z^*_K, z^*), predict the solution to time $t_{K+N_{lim}}$ where
$\sigma^2_{K+N_{lim}}(z^*_K, z^*) = \min_{z_K} \max_{z} \sigma^2_{K+N_{lim}}(z_K, z) \geq \sigma^2_{lim}$;

(6) Reinitialize time $t_K = t_{K+N_{lim}}$ and return to (1) for next measurement. (5.72)

All of the results for the monitoring problem with bound on error in the state estimate apply here as well, permitting statement of the final result for the monitoring problem with bound on error in the output estimate:

> Conclusion XII. For the case of infrequent sampling, the complete solution of the optimal monitoring design problem with bound on error in the output estimate — the determination of the optimal number of samplers to use at each measurement, their optimal locations, the optimal choice of measurement instrument accuracies and the position of maximum variance in the output estimate at each measurement — may be obtained at the first measurement time with the same design being optimal for all other measurement times. (C.XII)

5.4.2 Determination of the Position of Maximum Variance in the Output Estimate — In the solution procedure (5.72), steps (3) and (4) must be developed. First, from the form of $\underset{\sim}{\Phi}$,

$$1 = \phi_{11} > \phi_{22} > \phi_{22} > \ldots > \phi_{nn} > 0, \tag{5.73}$$

as seen in (5.15). Thus, in the determination of the number of terms necessary in the computation of the matrix convolution $[\underset{N}{\Omega}]$ in (3), from (5.70) and (5.20), the critical terms in the matrix, those which approach

their steady-state values slower than all the others, can be seen to be $[\underset{N}{\Omega}]_{12}$ and $[\underset{N}{\Omega}]_{21}$, where, from (5.70),

$$[\underset{N}{\Omega}]_{ij} \equiv [\Omega]_{ij} \sum_{n=1}^{N} \phi_{ii}^{n-1}\phi_{jj}^{n-1}. \tag{5.74}$$

As a measure of how rapidly the series in (5.74) grows as N increases, define

$$\rho_{ij}^{N} \equiv \frac{\phi_{ii}^{N-1}\phi_{jj}^{N-1}}{\phi_{ii}\phi_{jj}} \tag{5.75}$$

as the ratio of the contribution to the series for $[\underset{N}{\Omega}]_{ij}$ due to step N compared to the contribution from step 1 in the series. Thus, a meaningful check for approaching the steady-state value of the convolution is to find N sufficiently large that

$$\rho_{ij}^{N} \leq \varepsilon; \qquad i,j = 1,2,\ldots,n, \quad i = j \neq 1, \tag{5.76}$$

where ε is some practical convergence criterion.

Since $\underset{\sim}{\Omega}$ itself is a covariance matrix (see Appendix B), it is positive-definite; hence $[\Omega]_{12} = [\Omega]_{21}$. Thus it can be readily seen from (5.73), (5.74), and (5.75) that the series for terms $[\underset{N}{\Omega}]_{12}$ and $[\underset{N}{\Omega}]_{21}$ grow more slowly than all the others (excluding, of course, $[\underset{N}{\Omega}]_{11}$) since

$$\rho_{12}^{N} = \rho_{21}^{N} > \rho_{ij}^{N}, \qquad \text{all other } (i,j). \tag{5.77}$$

Thus, a convenient measure for the convergence

$$\lim_{N\to\infty} [\underset{N}{\Omega}] = [\underset{SS}{\Omega}]$$

is, simply, to find for just the second element of $\underset{\sim}{\Phi}$, ϕ_{22}, that value of N such that, for some convergence accuracy ε,

$$\rho_{12}^{N} \equiv \frac{\phi_{11}^{N-1}\phi_{22}^{N-1}}{\phi_{11}\phi_{22}} = \frac{\phi_{22}^{N-1}}{\phi_{22}} = \phi_{22}^{N-2} < \varepsilon. \tag{5.78}$$

Thus, for the infrequent sampling approximations to apply within some tolerance ε, at least N time steps must occur between sample times so that steady-state conditions are adequately approached.

In order to find the maximum in step (4), that is, find z* such that $\underset{\sim}{c}(z)^T \underset{\sim}{\Omega}_{SS} \underset{\sim}{c}(z)$ is maximized, an analytical approach is first sought. Since the problem is a simple extremization of a scalar-valued function of a single variable, elementary calculus techniques apply so that for some value of z_K a necessary condition for an extremum is

$$\frac{\partial}{\partial z} \sigma^2_{K+N}(z_K, z) = 0. \tag{5.79}$$

From Conclusion IX and (5.69)

$$\frac{\partial}{\partial z} \sigma^2_{K+N}(z_K, z) \doteq \frac{\partial}{\partial z} \left\{ \left[P^K_K(z_K) \right]_{11} + \cancel{N[\Omega]_{11}} + \underset{\sim}{c}(z)^T \underset{SS}{\Omega} \underset{\sim}{c}(z) \right\}$$

$$= \left(\frac{\partial}{\partial z} \underset{\sim}{c}(z)^T \right) \underset{SS}{\Omega} \underset{\sim}{c}(z) + \underset{\sim}{c}(z)^T \underset{SS}{\Omega} \left(\frac{\partial}{\partial z} \underset{\sim}{c}(z) \right). \tag{5.80}$$

Recalling that since Ω is a covariance matrix,

$$\Omega = \Omega^T,$$

$$\underset{SS}{\Omega} = \underset{SS}{\Omega}^T,$$

so that

$$\frac{\partial}{\partial z} \sigma^2_{K+N}(z_K, z) \doteq 2 \left(\frac{\partial}{\partial z} \underset{\sim}{c}(z)^T \right) \underset{SS}{\Omega} \underset{\sim}{c}(z).$$

Since

$$\underset{\sim}{c}(z)^T \equiv \left[1, \cos\left(\frac{\pi}{2L} z \right), \cos\left(2 \frac{\pi}{2L} z \right), \ldots \right],$$

$$\frac{\partial}{\partial z} \underset{\sim}{c}(z)^T = \left[0, -\frac{\pi}{2L} \sin\left(\frac{\pi}{2L} z \right), -2 \frac{\pi}{2L} \sin\left(2 \frac{\pi}{2L} z \right), \ldots \right].$$

Thus,

$$\frac{\partial}{\partial z}\sigma^2_{K+N}(z_K,z) = 2\sum_{i=1}^{n}\sum_{j=1}^{n} -(i-1)\frac{\pi}{2L}\sin\left[(i-1)\frac{\pi}{2L}z\right]\cos\left[(j-1)\frac{\pi}{2L}z\right]\left[\Omega_{SS}\right]_{ij} . \qquad (5.81)$$

For an extremum in $\sigma^2_{K+N}(z_K,z)$, set (5.81) to zero, from which it is seen clearly that for finding the solutions of (5.79), *analytical methods are of little use.*

The numerical solution of (5.79) using (5.81) and (5.69), however, is straightforward. Since the derivative can be so concisely written, it is well known that solving for the roots of (5.79), then checking the value of the function (5.69) at each root so as to classify each extrema in order to arrive at the global maximum is superior to direct one dimensional search methods (such as golden section or Fibonacci search) which do not employ derivatives (see [20] and [53]). Thus, any of the widely available root solving methods for nonlinear equations could be suitable for the determinization of z^* at the maximum of $\sigma^2_{K+N}(z_K,z)$ (see, for example, [61]).

5.5 Diffusive Systems Including Scavenging

Return now to the original problem of monitoring diffusive pollutant dispersal including environmental degradation or scavenging of the pollutant. The relevant transport equation, from (3.3), is given as

$$\frac{\partial \xi}{\partial t} = K\nabla^2\xi - \alpha\xi + f, \qquad (5.82)$$

where α is a smaller parameter. This equation describes diffusion in an arbitrary homogeneous region P where the small term $-\alpha\xi$ accounts for the scavenging of the pollutant from the medium. The scavenging term is typically much smaller than either the source or diffusion terms and usually leads to a slowly-changing component in the system response.

Application of separation of variables to the homogeneous form of (5.82) leads to the following state and Helmholtz equations:

$$\dot{x}(t) + (\lambda + \alpha)x(t) = 0, \tag{5.83}$$

$$\nabla^2 e(P) + \frac{\lambda}{K} e(P) = 0. \tag{5.84}$$

Comparison with equations (3.11) and (3.12) for the case of simple diffusion, the case in (3.4) with $\alpha \equiv 0$, shows that the *only* difference in the associated eigenproblem is in the rates of response in the *time* equation. The equation regarding the spatial response is identical with that for the case of simple diffusion. Thus, *all* the eigenvalues are seen to be shifted by the same amount α, the value of the scavenging parameter itself.

Notice that nothing has been said that restricts this result to specific coordinate systems, boundary conditions, etc. It is a general relationship between the eigensystems of (3.4) and (5.82). Thus, the modal state equations for the case with scavenging may be written

$$\dot{x}_n(t) = -(\lambda_n + \alpha)x_n(t) + f_n(t), \qquad n = 1,2,\ldots, \tag{5.85}$$

where $f_n(t)$ is the modal input to mode n (see (3.19)). Comparison of (5.85) with (3.20) for the case of simple diffusion shows that the problem with scavenging changes the response of the system with no-flow boundary conditions to that of a problem which lies somewhere between simple diffusion with no-flow boundary conditions and simple diffusion with fixed boundary conditions. It would seem from what we have seen in the infrequent sampling problem thus far that for the cases where α is small in (5.82), extensions of the earlier results of this chapter to the problem including scavenging should be possible.

Another way of seeing how the inclusion of the term $-\alpha\xi$ in (5.82) effects the structure of the eigenproblem associated with (5.82) can be shown by reconsidering the one-dimensional example of Section 3.2. Consider here only the homogeneous response. Thus, the problem may be stated as follows:

$$\frac{\partial \xi(z,t)}{\partial z} = K \frac{\partial^2 \xi(z,t)}{\partial z^2} - \alpha \xi(z,t); \tag{5.86}$$

$$\frac{\partial \xi(0,t)}{\partial z} \equiv 0, \qquad \frac{\partial \xi(2L,t)}{\partial z} \equiv 0; \tag{5.87}$$

$$\xi(z,0) \equiv \xi_0(z). \tag{5.88}$$

Now, make the transformation (see Mac Robert [82], p. 33)

$$\xi(z,t) \equiv \eta(z,t)e^{-\alpha t}. \tag{5.89}$$

Substitute (5.89) into (5.86) to obtain

$$\eta(z,t)\left[-\alpha e^{-\alpha t}\right] + \frac{\partial \eta(z,t)}{\partial t} e^{-\alpha t} = K \frac{\partial^2 \eta(z,t)}{\partial z^2} e^{-\alpha t} - \alpha \eta(z,t) e^{-\alpha t}, \tag{5.90}$$

which reduces to

$$\frac{\partial \eta(z,t)}{\partial t} = K \frac{\partial^2 \eta(z,t)}{\partial z^2}. \tag{5.91}$$

But the eigensystem for (5.91) given boundary conditions (5.87) is just that for the problem of simple diffusion already discussed in Section 3.2 from which the homogeneous solution may be written as

$$\eta(z,t) = \sum_{n=1}^{\infty} x_n(0)\, e^{-K(n-1)^2 \frac{\pi^2}{4L^2}} \cos\left((n-1)\frac{\pi}{2L} z\right) \tag{5.92}$$

where the initial conditions for the modes are given by

$$x_n(0) \equiv \int_0^{2L} \xi_0(z) \cos\left((n-1)\frac{\pi}{2L} z\right) dz. \tag{5.93}$$

Substitution of (5.93) into (5.89) then yields the important result for the case including scavenging

$$\xi(z,t) = e^{-\alpha t} \sum_{n=1}^{\infty} x_n(0)\, e^{-K(n-1)^2 \frac{\pi^2}{4L^2} t} \cos\left((n-1)\frac{\pi}{2L} z\right)$$

$$= \sum_{n=1}^{\infty} x_n(0)\, e^{-\left\{K(n-1)^2 \frac{\pi^2}{4L^2} + \alpha\right\} t} \cos\left((n-1)\frac{\pi}{2L} z\right). \tag{5.94}$$

Thus the solution to the problem including scavenging has exactly the *same eigenfunctions* as the case without scavenging and a set of *shifted eigenvalues* each of whose elements is just that of the problem without scavenging shifted by an amount α.

5.5.1 The Infrequent Sampling Problem — Consider a one-dimensional diffusive system described as follows:

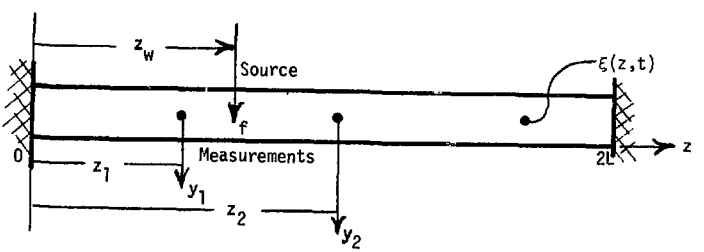


Figure 5.4

$$\frac{\partial \xi(z,t)}{\partial t} = \frac{\partial^2 \xi(z,t)}{\partial z^2} - \alpha \xi(z,t) + f(z,t); \tag{5.95}$$

$$\frac{\partial \xi(0,t)}{\partial z} = 0, \qquad \frac{\partial \xi(2L,t)}{\partial z} = 0; \tag{5.96}$$

$$\xi(z,0) = \xi_0; \tag{5.97}$$

$$f(z,t) \equiv w(t)\delta(z_w - z),$$

$$E[w(t)] = 0,$$

$$E[w(t)w(\tau)] = W\delta(t - \tau). \tag{5.98}$$

After simplification of the series solution of the homogeneous problem in (5.94) to a finite number of terms, n, it can be seen from the form of (3.37) for the problem without scavenging that the following set of modal state equations results:

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \cdot \\ \cdot \\ \cdot \\ \dot{x}_n \end{bmatrix} = \begin{bmatrix} -\alpha & & & \bigcirc \\ & -\left(\frac{k\pi^2}{4L^2} + \alpha\right) & & \\ & & \ddots & \\ \bigcirc & & & -\left((n-1)^2 \frac{k\pi^2}{4L^2} + \alpha\right) \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix}$$

$$+ \begin{bmatrix} \frac{1}{2L} \\ \frac{1}{L}\cos\left(\frac{\pi}{2L} z_w\right) \\ \cdot \\ \cdot \\ \cdot \\ \frac{1}{L}\cos\left((n-1)\frac{\pi}{2L} z_w\right) \end{bmatrix} w(t), \tag{5.99}$$

with initial condition

$$x(0) = [\xi_0, 0, \ldots, 0]^T. \tag{5.100}$$

The measurement equation is exactly that of (3.39) for the case with no scavenging.

Thus, comparison of the dynamic matrix $\underline{A}$ for the case with no scavenging in (3.37) with that in (5.99) for the inclusion of the α-term shows the one major difference for the infrequent sampling problem. In the former, $[\underline{A}]_{11} = 0$ while in the latter, $[\underline{A}]_{11} = -\alpha \neq 0$. Thus, the first modal state variable will in general exhibit a relatively slow response governed by the term $e^{-\alpha t}$. The effect of the initial condition $x_1(0)$ will decay at that rate whereas it remained constant in the case with no scavenging. This leads to differences in the asymptotic properties of the solutions which are developed in the following.

Consider the time discretization of (5.99). The state-transition matrix $\underline{\Phi}$ given in (4.8) for the $\underline{A}$ matrix in (5.99) is

$$\underline{\Phi} = \begin{bmatrix} e^{-\alpha T} & & & \bigcirc \\ & e^{-\left(\frac{K\pi^2}{4L^2} + \alpha\right)T} & & \\ & & \ddots & \\ \bigcirc & & & e^{-\left((n-1)^2 \frac{K\pi^2}{4L^2} + \alpha\right)T} \end{bmatrix}, \tag{5.101}$$

where the integration step $T \equiv (t_{K+1} - t_K)$. Assume as before that the problem starts at time t_0 with initial estimation error covariance matrix given by $\underline{M}_0$. Assume further that at time t_K, the estimation error constraint is reached so that a measurement is necessary at time t_K. It

is required to design the measurement by finding the optimal measurement position vector $\underline{z}_K^*$ so that the time when the error constraint is next reached is maximized.

Consider the evolution of the predicted estimation error covariance matrix with time after the sample at t_K:

$$\underline{P}_{K+N}^{K}(\underline{z}_K^*) = \underline{\Phi}^N \underline{P}_K^K(\underline{z}_K^*)\underline{\Phi}^{N^T} + \sum_{n=1}^{N} \underline{\Phi}^{n-1}\underline{\Omega}\underline{\Phi}^{n-1^T}. \tag{5.102}$$

Expand the above as matrices as was done for the case with no scavenging in (5.17) to obtain

$$\underline{P}_{K+N}^{K}(\underline{z}_K^*) = \begin{bmatrix} \left[\underline{P}_K^K(\underline{z}_K^*)\right]_{11}\phi_{11}^{2N} & \left[\underline{P}_K^K(\underline{z}_K^*)\right]_{12}\phi_{11}^{N}\phi_{22}^{N} & \left[\underline{P}_K^K(\underline{z}_K^*)\right]_{13}\phi_{11}^{N}\phi_{33}^{N}\cdots \\ \left[\underline{P}_K^K(\underline{z}_K^*)\right]_{21}\phi_{22}^{N}\phi_{11}^{N} & \left[\underline{P}_K^K(\underline{z}_K^*)\right]_{22}\phi_{22}^{2N} & \cdots \\ \vdots & \ddots & \\ & & \left[\underline{P}_K^K(\underline{z}_K^*)\right]_{nn}\phi_{nn}^{2N} \end{bmatrix}$$

$$+ \begin{bmatrix} [\Omega]_{11}\sum_{n=1}^{N}\phi_{11}^{2(n-1)} & [\Omega]_{12}\sum_{n=1}^{N}\phi_{11}^{n-1}\phi_{22}^{n-1} & [\Omega]_{13}\sum_{n=1}^{N}\phi_{11}^{n-1}\phi_{33}^{n-1} \\ [\Omega]_{21}\sum_{n=1}^{N}\phi_{22}^{n-1}\phi_{11}^{n-1} & [\Omega]_{22}\sum_{n=1}^{N}\phi_{22}^{2(n-1)} & \cdots \\ \vdots & \ddots & \\ & & [\Omega]_{nn}\sum_{n=1}^{N}\phi_{nn}^{2(n-1)} \end{bmatrix} \tag{5.103}$$

Now, if α in (5.95) is sufficiently small, then the diagonal elements of $\underline{\Phi}$, called ϕ_{ii}, $i = 1,2,\ldots,n$, will be related in (5.103) by the following ordering property:

$$1 > \phi_{11}^N >> \phi_{22}^N > \ldots > \phi_{nn}^N > 0. \tag{5.104}$$

Using (5.104), the matrices in (5.103) may be approximated by the following expression for N large:

$$\begin{bmatrix} \\ \underline{P}_{K+N}^K(\underline{z}_K^*) \\ \\ \end{bmatrix} \simeq \begin{bmatrix} \left[\underline{P}_K^K(\underline{z}_K^*)\right]_{11}\phi_{11}^{2N} & \\ & \bigcirc \end{bmatrix} + \begin{bmatrix} [\underline{\Omega}]_{11}\sum_{n=1}^{N}\phi_{11}^{2(n-1)} & \\ & \bigcirc \end{bmatrix} + \begin{bmatrix} 0 & \\ & \underline{\Omega}_{SS} \end{bmatrix} \tag{5.105}$$

Comparison of (5.105) with (5.21) for the case with no scavenging shows the expected result that here, the asymptotic matrix solution approaches that of just the (1,1)-element of the matrix with time plus the steady-state matrix $\underline{\Omega}_{SS}$ due to the forcing function.

For the monitoring problem with bound on error in the state estimate, from (5.105) the trace of the estimation error covariance matrix is given by

$$\mathrm{Tr}\left[\underline{P}_{K+N}^K(\underline{z}_K^*)\right] \simeq \left[\underline{P}_K^K(\underline{z}_K^*)\right]_{11}\phi_{11}^{2N} + [\underline{\Omega}]_{11}\sum_{n=1}^{N}\phi_{11}^{2(n-1)} + \mathrm{Tr}[\underline{\Omega}_{SS}], \tag{5.106}$$

which is similar in form to (5.22) for the problem without scavenging. The only differences lie in the first two terms on the right hand sides of (5.22) and (5.106). Both pairs of terms describe the response of $\left[\underline{P}_{K+N}^K(\underline{z}_K^*)\right]_{11}$ with time. In the former case, the response is that of a ramp with slope $[\underline{\Omega}]_{11}$ starting at $\left[\underline{P}_K^K(\underline{z}_K^*)\right]_{11}$. In the latter case, the

response starts from the same value but then slowly approaches a finite steady-state value in the limit as $N \to \infty$ much like all the other terms do in the matrix. The main difference is that the (1,1)-element of $\underset{\sim}{P}^{K}_{K+N}(\underset{\sim}{z}^{*}_{K})$ grows much, much slower to its final value than all the other elements of $\underset{\sim}{P}^{K}_{K+N}(\underset{\sim}{z}^{*}_{K})$; this is the result of requiring the scavenging parameter α to be small, leading to property (5.104).

A graphical depiction of the trace of (5.102) and its asymptotic approximation in (5.106) is shown in Figure 5.5. Comparison with Figure 5.2 for the case with no scavenging shows the difference in the asymptotic responses.

For the monitoring problem with bound on error in the output estimate, using the form for $\underset{\sim}{P}^{K}_{K+N}(\underset{\sim}{z}^{*}_{K})$ in (5.105) in the equation (5.68) developed earlier leads to

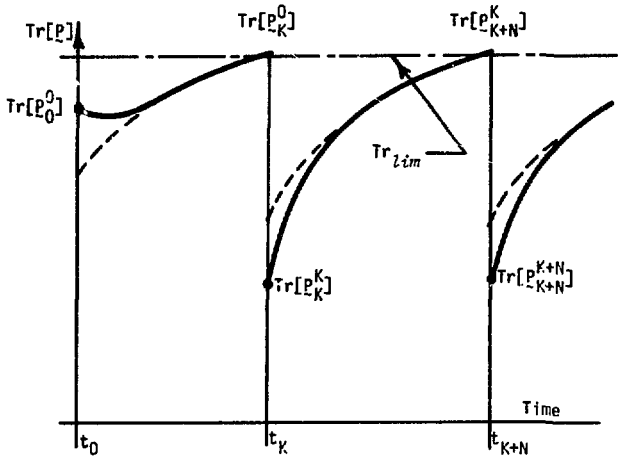
$$\sigma^{2}_{K+N}\left(\underset{\sim}{z}^{*}_{K},z\right) \simeq \left[\underset{\sim}{P}^{K}_{K}\left(\underset{\sim}{z}^{*}_{K}\right)\right]_{11}\phi^{2N}_{11} + [\underset{\sim}{Q}]_{11}\sum_{n=1}^{N}\phi^{2(n-1)}_{11} + \underset{\sim}{c}(\underset{\sim}{z})^{T}\underset{SS}{\underset{\sim}{Q}}\underset{\sim}{c}(z). \qquad (5.107)$$

Comparison of (5.107) with (5.69) for the case with no scavenging shows the same asymptotic properties as exhibited in the problem with bound on error in the state estimate above which leads to the general result for the problem with scavenging:

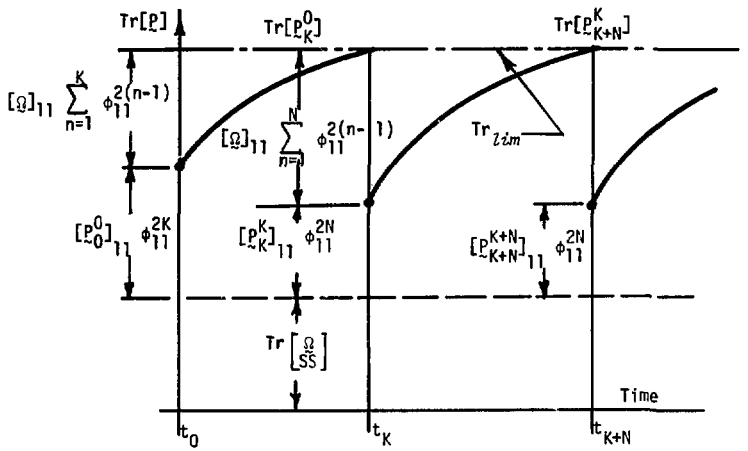
> Conclusion XIII. For diffusive systems with scavenging, all the results for the infrequent sampling problem for normal diffusion apply directly so long as the scavenging parameter is sufficiently small. (C.XIII)

5.6 One-Dimensional Diffusion with Fixed Boundary Conditions

Consider the case of a one-dimensional diffusive system with the pollutant concentrations at the ends of the medium fixed at known values throughout the time interval of interest. This case was modeled in



(A) Actual response



(B) Asymptotic approximation

Figure 5.5. The infrequent sampling problem for systems with scavenging; compare to Figure 5.2 for systems with no scavenging.

Section 3.2 2. Such systems are of much lesser practical importance than those with no-flow boundary conditions since it is difficult to find many physical situations of any significance where fixed end conditions occur (see Brewer [22] and Young [131]).

For such a system, the following state and measurement equations apply:

$$\dot{\underline{x}} = \underline{A}\underline{x} + \underline{D}\underline{w}, \tag{5.108}$$

$$\underline{y} = \underline{C}\underline{x} + \underline{v}, \tag{5.109}$$

where, from (3.56),

$$\underline{A} \equiv \begin{bmatrix} -\frac{K\pi^2}{4L^2} & & & \bigcirc \\ & -4\frac{K\pi^2}{4L^2} & & \\ & & \ddots & \\ \bigcirc & & & -(n)^2\frac{K\pi^2}{4L^2} \end{bmatrix}, \quad \underline{D} \equiv \begin{bmatrix} \frac{1}{L}\sin\left(\frac{\pi}{2L}z_{w_1}\right) \cdots \\ \frac{1}{L}\sin\left(2\frac{\pi}{2L}z_{w_1}\right) \\ \vdots \\ \frac{1}{L}\sin\left(n\frac{\pi}{2L}z_{w_1}\right) \cdots \end{bmatrix},$$

$$\underline{C} \equiv \begin{bmatrix} \sin\left(\frac{\pi}{2L}z_1\right) & \sin\left(2\frac{\pi}{2L}z_1\right) \cdots \\ \sin\left(\frac{\pi}{2L}z_2\right) \cdots \end{bmatrix}. \tag{5.110}$$

From the definition of $\underline{A}$ above and $\underline{\Phi}$ in (4.8) and (4.9), the state transition matrix for fixed boundary concentrations is given as follows where the time step $T \equiv \left(t_{K+1} - t_K\right)$:

$$\Phi \equiv e^{\underline{A}T} = \begin{bmatrix} e^{-\frac{K\pi^2}{4L^2}T} & & & \\ & e^{-4\frac{K\pi^2}{4L^2}T} & & \\ & & \ddots & \\ & & & e^{-(n)^2\frac{K\pi^2}{4L^2}T} \end{bmatrix} . \qquad (5.11)$$

Comparing this transition matrix with that from the case for no-flow boundary conditions (see (5.15)) shows how the fundamental difference in the two normal mode expansions effects the dynamical responses of such systems. In the case with no-flow boundary conditions $[\underset{\sim}{\Phi}]_{11} = 1$, whereas for the case with fixed concentrations at the boundaries, $0 < [\underset{\sim}{\Phi}]_{11} < 1$.

This difference manifests itself in ways which effect both the monitoring problems with bound on error in the state and output estimates. Consider the predicted covariance matrix equation from time t_K to time t_{K+N}:

$$\underset{\sim}{P}^{K}_{K+N} = \underset{\sim}{\Phi}^{N}\underset{\sim}{P}^{K}_{K}\underset{\sim}{\Phi}^{N^T} + \sum_{n=1}^{N} \underset{\sim}{\Phi}^{n-1}\underset{\sim}{\Omega}\underset{\sim}{\Phi}^{n-1^T} . \qquad (5.10)$$

From (5.111), let

$$[\underset{\sim}{\Phi}]_{ii} \equiv \Phi_{ii}, \qquad i = 1,2,\ldots,n. \qquad (5.112)$$

Then, (5.10), may be expanded as follows:

$$\underline{P}^K_{K+N} = \begin{bmatrix} \left[\underline{P}^K_K\right]_{11}\phi_{11}^{2N} & \left[\underline{P}^K_K\right]_{12}\phi_{11}^{2}\phi_{22}^{2} \cdots \\ \left[\underline{P}^K_K\right]_{21}\phi_{22}^{N}\phi_{11}^{N} & \left[\underline{P}^K_K\right]_{22}\phi_{22}^{2N} \\ \vdots & \ddots \end{bmatrix} + \begin{bmatrix} [Q]_{11}\sum_{n=1}^{N}\phi_{11}^{2(n-1)} & [Q]_{12}\sum_{n=1}^{N}\phi_{11}^{n-1}\phi_{22}^{n-1} \cdots \\ [Q]_{21}\sum_{n=1}^{N}\phi_{22}^{n-1}\phi_{11}^{n-1} & [Q]_{22}\sum_{n=1}^{N}\phi_{22}^{2(n-1)} \\ \vdots & \ddots \end{bmatrix} \quad (5.113)$$

Comparing (5.113) with (5.17) for the case with no-flow boundary conditions shows that the properties of first elements of both matrices in (5.17) which proved to be crucial to the simplicity found in the infrequent sampling problem do *not* hold in the case with fixed end concentrations.

However, as in the case with scavenging, notice that owing to the ordering of the eigenvalues in the $\underline{A}$ matrix in (5.110), there is a corresponding ordering in the elements of $\underline{\Phi}$ such that for $\underline{P}^K_{K+N}$ in (5.113),

$$1 > \phi_{11}^N > \phi_{22}^N > \ldots > \phi_{nn}^N > 0. \quad (5.114)$$

Notice from the matrix $\underline{A}$ that for the first two terms,

$$4\lambda_1 = \lambda_2 \quad (5.115)$$

so that the second mode decays four times faster than the first. Thus, the two dominant eigenvalues are widely enough separated to proceed with approximations for an infrequent sampling problem.

Use (5.112) in (5.113) to obtain

$$\begin{bmatrix} \\ \underline{P}^K_{K+N} \\ \\ \end{bmatrix} = \begin{bmatrix} \left[\underline{P}^K_K\right]_{11}\phi_{11}^{2N} & \\ \bigcirc & \end{bmatrix} + \begin{bmatrix} [Q]_{11}\sum_{n=1}^{N}\phi_{11}^{2(n-1)} & \\ \bigcirc & \end{bmatrix} + \begin{bmatrix} 0 & \\ & \underline{Q}_{SS} \end{bmatrix}. \quad (5.116)$$

which is exactly the same result as in (5.105) for the case with scavenging. The trace of (5.116) follows the form of (5.106) for the scavenging problem so that for the monitoring problem with bound on error in the state estimate, all the results for the infrequent sampling problem apply. Trajectories for $\mathrm{Tr}[\underset{\sim}{P}^K_{K+N}(\underset{\sim}{z}^*_K)]$ would appear similar to those for the problem of no-flow boundary conditions including scavenging as shown in Figure 5.5; the rate of approach to steady-state for the (1,1)-element of $\underset{\sim}{P}^K_{K+N}$ would be faster if λ_1 for this problem is larger than α in the former problem.

For the monitoring problem with bound on the error in the output estimate, the case of fixed boundary conditions causes a confusing relationship in the minimax problem for finding the location of maximum variance in the output estimate. From the approximation for $\underset{\sim}{P}^K_{K+N}$ in (5.116),

$$
\begin{aligned}
\sigma^2_{K+N}(\underset{\sim}{z}_K, z) \;&\leq\; \underset{\sim}{c}(z)^T \underset{\sim}{P}^K_{K+N}(\underset{\sim}{z}_K)\underset{\sim}{c}(z) \\
&\approx \left[\sin\left(\tfrac{\pi}{2L}z\right)\ \sin\left(2\tfrac{\pi}{2L}z\right)\ \cdots\right]
\begin{bmatrix}
\left[\underset{\sim}{P}^K_K(\underset{\sim}{z}_K)\right]_{11}\phi_{11}^{2N} & & \\
& \bigcirc & \\
& & \\
& & \\
&

where $\underline{\varphi}(z)$ is derived from the definition of $\xi(z,t)$ in (3.48). Thus, for N large,

$$\sigma^2_{K+N}\left(\underline{z}_K,z\right) \simeq \sin^2\left(\frac{\pi}{2L}z\right)\left[\underline{P}^K_K\left(\underline{z}_K\right)\right]_{11}\phi^{2N}_{11} + \sin^2\left(\frac{\pi}{2L}z\right)[\underline{\Omega}]_{11}\sum_{n=1}^{N}\phi^{2(n-1)}_{11} + \underline{\varphi}(z)^T\underset{SS}{\underline{\Omega}}\,\underline{\varphi}(z), \tag{5.118}$$

which is of the form

$$\sigma^2_{K+N}\left(\underline{z}_K,z\right) = \alpha\left(\underline{z}_K,z,N\right) + \beta(z,N) + \varepsilon(z) \tag{5.119A}$$

$$= \alpha\left(\underline{z}_K\right)\beta(z)\gamma(N) + \beta(z)\delta(N) + \varepsilon(z). \tag{5.119B}$$

It is required to find $\underline{z}^*_K$ and z^* such that, for N large,

$$\sigma^2_{K+N}\left(\underline{z}^*_K,z^*\right) = \min_{\underline{z}_K}\max_{z}\sigma^2_{K+N}\left(\underline{z}_K,z\right). \tag{5.120}$$

From the separation of functions in (5.119B), it is clear that finding $\underline{z}^*_K$ should be done *exactly* as before, that is,

$$\text{Find } \underline{z}^*_K \text{ at } t_K \text{ such that } \left[\underline{P}^K_K\left(\underline{z}^*_K\right)\right]_{11} = \min_{\underline{z}_K}\left[\underline{P}^K_K\left(\underline{z}_K\right)\right]_{11}. \tag{5.121}$$

It would appear that knowing $\underline{z}^*_K$, the optimal measurement positions for the measurement at time t_K, one could then substitute its value directly into (5.118) to solve for the position of maximum variance, z^*, at time t_{K+N}. However, as seen in (5.119B), the terms (α β γ) and (β δ) are *functions of time* t_{K+N}, such that the relationship between ($\alpha\beta\gamma$ + $\beta\delta$) and (ε) in (5.119B) is always changing. A general statement of a separation principle like (5.69) for systems with no-flow boundary conditions cannot be made for the case with fixed boundary conditions. However, if more knowledge exists about the specific problem under study, for example, if in (5.118), $[\underline{\Omega}]_{11} >> [\underline{\Omega}]_{ij}$, i and j $\neq$ 1, then the term ($\beta\delta$) in (5.119B) may dominate the right-hand side of that equation for N large such that,

for such a special case,

$$\max_{z} \sigma^2_{K+N}\left(\underset{\sim}{z}^*_K, z\right) = \max_{z} \sin^2\left(\frac{\pi}{2L} z\right).$$

What is clear about the general case is that the minimax problem in (5.120) simplifies to (1) finding $\underset{\sim}{z}^*_K$ in the minimization in (5.21) as before then (2) evaluating the position z^* for the maximum $\sigma_{K+N}(\underset{\sim}{z}^*_K, z^*)$ in (5.118) iteratively as N increases until for some $t_{K+N_{lim}}$, $\sigma^2_{K+N}(\underset{\sim}{z}^*_K, z^*) \geq \sigma^2_{lim}$. The latter procedure is *greatly simplified* using the approximations of the infrequent sampling problem as can be seen by comparing the simplicity of the expression for σ^2_{K+N} in (5.118) with the complicated expression that would have resulted had the full matrices for $\underset{\sim}{P}^K_{K+N}$ in (5.113) been involved instead.

Thus, results for the infrequent monitoring problem with no-flow boundary conditions extend with restrictions to the case with fixed boundary conditions.

> Conclusion XIV. For N large, all the results for the infrequent sampling problem with no-flow boundary conditions with bound on error in the *state* estimate extend to the case with fixed boundary conditions. The results for bound on error in the *output* estimate *do not* all extend to the case with fixed boundary conditions in general; however, application of the infrequent sampling problem approximations *does drastically simplify* solution of the functionally interdependent minimax problem to the solution of two independent problems in minimization and maximization. (C.XIV)

5.7 Extension to Monitoring Problems in Three Dimensions: Systems with Emission Boundary Conditions

As a means of demonstrating the power of the results for the infrequent sampling problem, consider extensions to diffusive systems in three dimensions; examples of applications might include pollutant transport in estuaries or bays and radiation level detection in settling basins

or in groundwater systems. Suppose there is a rectangular three-dimensional region into which known stochastic sources are injecting pollutant. In the case of bay, estuary or settling basin systems, the upper surface of this region would interface with the earth's atmosphere whereas in groundwater applications, the upper surface of this hypothetical region could coincide with the local level of the water table. The requirement of the problem is to place the fewest number of sampling stations at the best locations *on the surface* of the region, taking the fewest number of samples over a given time interval in order to maintain the error in the estimate of the concentration *throughout* the three-dimensional volume below a given bound. This is an interesting variation of the general problem in three dimensions where sources may occur anywhere in the volume but measurements are required to be taken only on one surface of the volume.

The validity of the description of pollutant transport in such systems by the use of Fickian diffusion has not been thoroughly studied. However, it seems reasonable to assume that if small enough subregions, which may be called "components," are considered, then coupling large numbers of such component subregions together, each of which is governed by its own diffusion equation, could result in a system of submodels which could be used to model a large, possibly inhomogeneous, anisotripic medium. Thus, this example is presented for its conceptual interest as a starting point toward a more sophisticated approach to solutions for pollutant monitoring problems of this type.

Assume the component subregion is described schematically as in Figure 5.6. One of the r generalized sources, $w_i(t)$, is shown somewhere in the volume with its position vector defined as

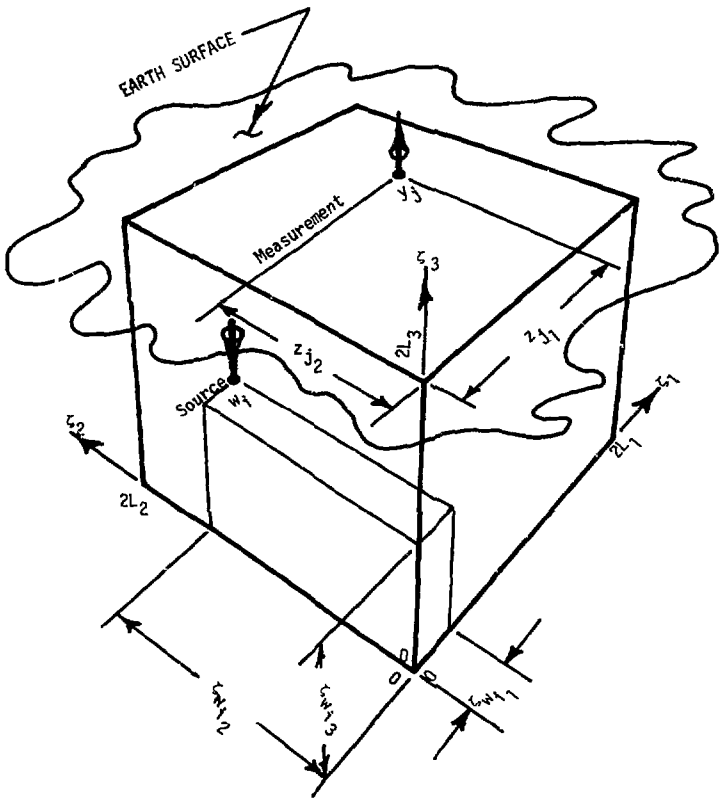


Figure 5.6. Three-dimensional component subregion for a three-dimensional monitoring problem.

$$\underline{\zeta}_{w_i} \equiv \left[\zeta_{w_{i_1}}, \zeta_{w_{i_2}}, \zeta_{w_{i_3}}\right]^T, \qquad i = 1,2,\ldots,r, \qquad (5.122)$$

One of the set of m generalized measurements y_j is shown on the surface with its position given by

$$\underline{z}_j \equiv \left[z_{j_1}, z_{j_2}, 2L_3\right]^T, \qquad j = 1,2,\ldots,m, \qquad (5.123)$$

If the size of the rectangular region is sufficiently small, the diffusivity throughout the medium may be approximated as a constant. The boundary conditions of the submerged surfaces are chosen to be of no-flow type so that other such components may be coupled together in order to approximate inhomogeneous material properties over larger regions (see Young [131], Chap. 3).

At the upper surface of the component, the assumption is made that a no-flow boundary condition adequately models the characteristics of the pollutant exchange across the upper boundary of the region. In problems involving transport of a volatile soluble contaminant in water systems (like DDT or disolved radioactive wastes), this assumption could be changed, for instance, to include emission of the pollutant into the atmosphere at the earth's surface. An approximate model of such emission is Robin's boundary condition (see Berg and Mc Gregor [18], Sections 3.6 and 4.9, Mac Robert [82], p. 28 and Duff and Naylor [34], Section 7.3). The only difference such a modification makes in the normal mode analysis is in the eigensystem which results for the ζ_3 coordinate direction, which is similar in form to that for no-flow boundary conditions but has interesting conceptual differences (see [18], Section 4.9).

Suppose the initial pollutant concentration throughout the medium is given by the function $\xi_0(\zeta)$. Thus, the initial-boundary value problem for this system is defined as follows:

$$\frac{\partial \xi}{\partial t} = K\left(\frac{\partial^2 \xi}{\partial \zeta_1^2} + \frac{\partial^2 \xi}{\partial \zeta_2^2} + \frac{\partial^2 \xi}{\partial \zeta_3^2}\right) + f(\underset{\sim}{\zeta},t); \tag{5.124}$$

$$\frac{\partial \xi}{\partial \zeta_1} = 0, \qquad \zeta_1 = 0, \qquad \zeta_1 = 2L_1, \tag{5.125A}$$

$$\frac{\partial \xi}{\partial \zeta_2} = 0, \qquad \zeta_2 = 0, \qquad \zeta_2 = 2L_2, \tag{5.125B}$$

$$\frac{\partial \xi}{\partial \zeta_3} = 0, \qquad \zeta_3 = 0, \qquad \zeta_3 = 2L_3; \tag{5.125C}$$

$$\xi(\underset{\sim}{\zeta},0) \equiv \xi_0(\underset{\sim}{\zeta}); \tag{5.126}$$

$$f_i\left(\underset{\sim}{\zeta}_{w_i},t\right) \equiv w_i(t)\delta\left(\zeta_1 - \zeta_{w_{i_1}}\right)\delta\left(\zeta_2 - \zeta_{w_{i_2}}\right)\delta\left(\zeta_3 - \zeta_{w_{i_3}}\right),$$

$$E\left[w_i(t)\right] = 0,$$

$$E\left[w_i(t)w_i(\tau)\right] = W_i\delta(t - \tau), \qquad i = 1,2,\ldots,p. \tag{5.127}$$

The no-flow boundary conditions are specified for all surfaces by (5.125). The initial condition as a function of the spatial coordinate vector $\underset{\sim}{\zeta}$ is given in (5.126), while the stochastic point sources with their statistics are described in (5.127).

The essential difference between this problem and the two-dimensional case treated in Section 3.3 is in the extension to eigensystems in three dimensions and the resultant increase in dimensionality as mentioned in Section 3.4.

Begin the analysis by assuming a solution in separated variables of the form

$$\xi(\underset{\sim}{\zeta},t) = \sum_{\ell=1}^{\infty}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty} x_{\ell mn}(t)\, e_{\ell mn}(\underset{\sim}{\zeta})$$

$$= \sum_{\ell=1}^{\infty}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty} x_{\ell mn}(t)\, e_\ell(\zeta_1)\, e_m(\zeta_2)\, e_n(\zeta_3). \tag{5.128}$$

From the one- and two-dimensional problems in Chapter 3, eigensystems for the coordinates ζ_1, ζ_2, and ζ_3, given boundary conditions (5.125), can be written down immediately as follows:

$$\lambda_\ell = \frac{1}{R_\ell C_\ell}, \qquad \ell = 1,2,\ldots, \tag{5.129A}$$

$$e_\ell(\zeta_1) = \cos\ (\ell - 1)\frac{\pi}{2L_1}\zeta_1\ ; \tag{5.129B}$$

$$\lambda_m = \frac{1}{R_m C_m}, \qquad m = 1,2\ldots., \tag{5.130A}$$

$$e_m(\zeta_2) = \cos\ (m - 1)\frac{\pi}{2L_2}\zeta_2\ ; \tag{5.130B}$$

$$\lambda_n = \frac{1}{R_n C_n}, \qquad n = 1,2,\ldots, \tag{5.131A}$$

$$e_n(\zeta_3) = \cos\ (n - 1)\frac{\pi}{2L_3}\zeta_3\ . \tag{5.131B}$$

The generalized modal resistances and capacitances, the R's and C's above, are exactly those given for the two-dimensional case in (3.61). As before, substitution of $\xi(\underset{\sim}{\zeta},t)$ in (5.128) into the differential equation (5.124), right-multiplying by eigenfunctions, integrating over the volume and applying orthogonality results in the following generalized normal mode state equation:

$$\dot{x}_{\ell mn}(t) = -\left(\frac{1}{R_\ell C_\ell} + \frac{1}{R_m C_m} + \frac{1}{R_n C_n}\right)x_{\ell mn}(t) + \frac{1}{C_\ell C_m C_n}\int_{\zeta_1=0}^{2L_1}\int_{\zeta_2=0}^{2L_2}\int_{\zeta_3=0}^{2L_3} f(\underset{\sim}{\zeta},t)\cos\left((\ell-1)\frac{\pi}{2L_1}\zeta_1\right)\cos\left((m-1)\frac{\pi}{2L_2}\zeta_2\right)\cos\left((n-1)\frac{\pi}{2L_3}\zeta_3\right)d\zeta_3 d\zeta_2 d\zeta_1. \tag{5.132}$$

The initial conditions for $\underset{\sim}{x}(t)$ are found as follows from (5.126) and (5.128),

$$\xi_0(\underset{\sim}{\zeta}) \equiv \sum_{\ell=1}^{\infty}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty} x_{\ell mn}(0)\, e_\ell(\zeta_1)\, e_m(\zeta_2)\, e_n(\zeta_3). \tag{5.133}$$

If $\xi_0(\underset{\sim}{\zeta})$ is expandable in a triple Fourier series, then $x_{\ell mn}(0)$ is given

as follows (see Mac Robert [82], p. 43):

$$x_{\ell mn}(0) = \frac{1}{C_\ell C_m C_n} \int_{\zeta_1=0}^{2L_1} \int_{\zeta_2=0}^{2L_2} \int_{\zeta_3=0}^{2L_3} \xi_0(\underline{\zeta})\, e_\ell(\zeta_1)\, e_m(\zeta_2)\, e_n(\zeta_3)\, d\zeta_3 d\zeta_2 d\zeta_1 \qquad (5.134)$$

where the eigenfunctions are given in (5.129) through (5.131).

The stochastic point sources are transformed into modal inputs in a similar fashion:

$$\frac{1}{C_\ell C_m C_n} \int_{\zeta_1=0}^{2L_1} \int_{\zeta_2=0}^{2L_2} \int_{\zeta_3=0}^{2L_3} f(\underline{\zeta},t)\, e_\ell(\zeta_1)\, e_m(\zeta_2)\, e_n(\zeta_3) d\zeta_3 d\zeta_2 d\zeta_1$$

$$= \left[\frac{1}{C_\ell C_m C_n} e_\ell\left(\zeta_{w_{i_1}}\right) e_m\left(\zeta_{w_{i_2}}\right) e_n\left(\zeta_{w_{i_3}}\right) \right] w_i(t) \qquad i = 1,2,\ldots,r, \qquad (5.135)$$

where, treating the point sources as distributions, the eigenfunctions in (5.135) are evaluated at the coordinate positions of the i*th* point source.

Truncating the triple Fourier series in (5.128) and retaining n terms in each results in a set of state and measurement equations entirely analogous to those for the two-dimensional problem in Section 3.3. The diagonal element for A for the (i,j,k)-*th* equation is

$$-\lambda_{ijk} = -\left(\frac{1}{R_i C_i} + \frac{1}{R_j C_j} + \frac{1}{R_k C_k} \right), \qquad (5.136)$$

so that the eigenvalues of the three-dimensional problem are simply the *sums* of those for one-dimensional problems written in each of the three coordinate directions. Similarly (see (3.62) and (3.64)), the elements of the $\underset{\sim}{D}$ and $\underset{\sim}{C}$ matrices are merely triple *products* of the eigenfunctions. Thus, the similarity with the two-dimensional case is well established.

Notice that in the discretization of the elements of $\underset{\sim}{A}$ from (5.136) and Table (3.61), $[\underset{\sim}{A}]_{11} = 0$ so that $\phi_{11} = 1$; thus all the results for the infrequent sampling problem with *no-flow* boundary conditions extend

directly to multidimensional regions. Thus, regardless of the dimensionality of a region, if no-flow boundary conditions exist at all boundaries, the monitoring problem may be treated in a straight orward manner with the techniques of the infrequent sampling problem.

Consider the inclusion suggested earlier of the emission of pollutant into the atmosphere at the surface of the component subregion, at $\zeta_3 = 2L_3$. A model for such emission (see Mac Robert [82], p. 28) is given by the following homogeneous boundary condition:

$$\frac{\partial \xi(\underset{\sim}{\zeta},t)}{\partial \zeta_3} + h\left[\xi(\underset{\sim}{\zeta},t) - \xi_3(\zeta_1,\zeta_2)\right] = 0; \qquad \zeta_3 = 2L_3, \quad (5.137)$$

where ξ_3 is the pollutant concentration in the atmosphere over the surface $\zeta_3 = 2L_3$, taken to be constant over time. Thus, the atmosphere acts like a pollutant source with constant concentration $\xi_3(\zeta_1,\zeta_2)$. h is a constant relating the emissivity of the surface e to the diffusivity within the component subregion by

$$h \equiv e/K. \qquad (5.138)$$

Berg and Mc Gregor([18], Section 4.9) show that the eigensystem for a one-dimensional system with a no-flow boundary condition like (5.123C) at $\zeta_3 = 0$ and a boundary condition with emission of the form (5.137) at $\zeta_3 = 2L_3$ can be described as follows.

$$\sqrt{\lambda_n} = (n - 1)\frac{\pi}{2L_3} + \mu_n, \qquad n = 1,2,\ldots; \qquad (5.139A)$$

$$e_n(\zeta_3) = \cos\left[\left\{(n - 1)\frac{\pi}{2L_3} + \mu_n\right\}\zeta_3\right] \qquad (5.139B)$$

where $\sqrt{\lambda_n}$ must be a positive root of the transcendental equation

$$\sqrt{\lambda_n}\,\tan\left(2L_3\sqrt{\lambda_n}\right) = h. \qquad (5.139C)$$

A graphical solution of (5.139C) shows that there is an ordering of the roots $\sqrt{\lambda_n}$ such that, for μ_n,

$$\frac{\pi}{2} > \mu_1 > \mu_2 > \ldots > \mu_n > \mu_{n+1} > \ldots > 0. \tag{5.139D}$$

For example, for $2L_3 \equiv 1$ and $h \equiv 0.1$,

n	1	2	3	4	5
λ_n	0.3111	3.1731	6.2991	9.4333	12.5743

(5.139E)

Thus, it is found that an ordering in this problem exists such that, for λ_n,

$$0 > \lambda_1 > \lambda_2 > \ldots, \qquad n = 1,2,\ldots . \tag{5.139F}$$

Since the eigenvalues for the three-dimensional problem are the *sums* of those in eigenproblems written in the three independent coordinate directions ζ_1, ζ_2, and ζ_3, from (5.136) it is seen that if an emission boundary condition is used at $\zeta_3 = 2L_3$, the crucial first eigenvalue in the $\underline{A}$ matrix is given by

$$\lambda_{111} = \left(0 + 0 + \mu_1^2\right) \tag{5.140}$$

where μ_1^2 is the first eigenvalue for the modified eigensystem (5.139). This leads to an ordering for the $\underline{\Phi}$ matrix elements such that

$$1 > \phi_{11} > \phi_{22} > \ldots \tag{5.141}$$

so that the concepts developed for the infrequent sampling problems for the cases with fixed boundary conditions and scavenging apply here as well. It should be noted that since $\mu_1 > 0$, the first eigenfunction in (5.139B) will be a function of ζ_3 so that the minimax problem possesses

the modified separation property of (5.119) for the case of fixed boundary conditions. Thus, the case of practical interest accounting for emission at a boundary is seen to fall within the framework of the infrequent sampling problem.

> Conclusion XV. For N large, the results of Conclusion XIV for the case with fixed boundary conditions are seen to extend to regions with emission or radiation boundary conditions. (C.XV)

Another interesting point about the structure of this type of monitoring problem is that even though the dynamic response of the process must be computed for the entire region in three-space, the measurement position optimization is constrained to a two-dimensional subspace, that is, to the surface

$$\zeta_3 = 2L_3. \tag{5.142}$$

This reduces the domain of the optimization considerably and emphasizes the power and versatility of constrained optimization techniques. In Section 5.3.6, a first-order gradient technique with linear constraints was described. In the context of the problems of this section, the power of such a technique is demonstrated in being able to express the requirement (5.142) directly as an equality constraint upon the domain of ζ_3 in the optimization.

In the application to groundwater problems, a more practical problem statement might be to constrain measurements to be taken anywhere down to a depth ϵ below the upper surface of the component subregion, that is, to a depth ϵ below the water table. This form of a constraint is readily placed upon the domain of the optimized variables as follows (see (5.5.3)):

For the position of the jth measurement device, require that z_{j_3}, the element of $\underline{z}_j$ in the ζ_3 coordinate direction, be limited to

$$\left(2L_3 - \epsilon\right) \leq z_{j_3} \leq 2L_3 \qquad j = 1,2,\ldots,m; \tag{5.143}$$

the form of a constraint for the optimization algorithm must be

$$z \leq z_{max}; \tag{5.144}$$

thus, decompose the single inequality constraint in (5.143) into two of the form (5.144) to obtain

$$z_{j_3} \leq 2L_3,$$

$$-z_{j_3} \leq (2L_3 - \epsilon). \tag{5.145}$$

Thus, the subspace for the measurement position optimization consisting of a layer of depth ϵ beneath the surface of the region is entered into the optimization algorithm as two simple inequality constraints on the elements z_{j_3} given in (5.145).

Thus, formulation of a three-dimensional pollutant monitoring problem over a homogeneous region with various boundary conditions amounts to a straightforward extension of the methods used for one- and two-dimensional problems. In addition, confining the admissible region for optimal monitor placement is a natural application of constrained optimization techniques.

5.8 The Management Problem

Thus far, consideration has been given solely to the problem involved in the *design* of a measurement — the number and quality of measurement sensors and where they should be placed — in order to minimize the total number of samples necessary over some time interval. It is the requirement, on the other hand, of the *management* problem to determine at what times within that time interval the measurements should be made in order to minimize the total number of samples necessary overall.

It is desired to prove that the optimal management program is to sample *only* when the error criterion for the state or output estimate has reached its limit. In general, this is a difficult fact to establish. Results are clear for the scalar case, however, and (algebraically tedious) constructive proofs for a system with only two normal mode states and one measurement device indicate that such a sampling program is also optimal for the vector case. However, obtaining a comprehensive proof that sampling only at the limits is optimal for multidimensional normal mode representations remains an elusive task. Heuristically, the verifiable result for scalar systems still seems to be extendable to the multivariable case, as will be shown.

5.8.1 Optimality in the Scalar Case — Consider a scalar system whose Kalman Filter covariance equations (see Chapter 4, Figure 4.1) can be reduced to

$$p_{K+1}^{K} = \phi^2 p_K^K + \omega, \quad p_0^0 \equiv \mu_0; \tag{5.146}$$

$$p_{K+1}^{K+1} = p_{K+1}^{K}\left[\frac{\nu}{p_{K+1}^{K} c_{K+1}^2 + \nu}\right], \tag{5.147}$$

where ω and ν are the disturbance and measurement noise variances, p is the variance in $\hat{x}$ and c is the scalar measurement coefficient.

Assume the process starts at time t_0. In order to deduce the optimal sampling program, compare the two following monitoring programs which correspond to sampling at the error limit (2) and sampling before the error limit is reached (1):

(1) Predict to t_1, sample at time t_1 and predict ahead to t_N;
(2) Predict to t_N, then sample. (5.148)

The optimality of one program over the other will be established after time t_{K+N} by the determination of which of the two has the smaller

variance p, since both will have used the same number of measurements (one each).

As a starting point, make the assumption that the characteristics of the measurements at the two times (specified by c_{K+1}^2 and ν in (5.147)) are the same. The more general case where ν can vary and c_1^2 at t_1 in the first measurement program and c_N^2 at t_N in the second may be different is commented upon later. Thus, for now, let $c_1^2 = c_N^2 \equiv c^2$ at both samples.

Case (1)

(A) Predict from t_0 to t_1:

$$p_1^0 = \phi^2 \mu_0 + \omega; \tag{5.149}$$

(B) Sample at t_1:

$$p_1^1 = p_1^0 \left[\frac{\nu}{p_1^0 c^2 + \nu} \right]$$

$$= (\phi^2 \mu_0 + \omega) \left[\frac{\nu}{(\phi^2 \mu_0 + \omega) c^2 + \nu} \right]; \tag{5.150}$$

(C) Predict to t_N:

$$p_N^1 = (\phi^2)^{N-1} p_1^1 + \sum_{n=1}^{N-1} (\phi^2)^{n-1} \omega. \tag{5.151}$$

Case (2)

(A) Predict to t_N:

$$p_N^0 = (\phi^2)^N \mu_0 + \sum_{n=1}^{N} (\phi^2)^{n-1} \omega \tag{5.152A}$$

$$= (\phi^2)^{N-1} p_1^0 + \sum_{n=1}^{N-1} (\phi^2)^{n-1} \omega. \tag{5.152B}$$

(B) Sample at t_N:

$$p_N^N = p_N^0 \left[\frac{\nu}{p_N^0 c^2 + \nu} \right]. \tag{5.153}$$

It is required to show that in (5.148), program (2) is optimal (which is an analogous case to sampling at the limit in the monitoring problem when $p_N^0 \geq p_{lim}$, an error limit). This can be shown by finding conditions under which

$$p_N^N < p_N^1. \tag{5.154}$$

To illustrate the relationships involved in the optimality of such a monitoring program, consider Figure 5.7.

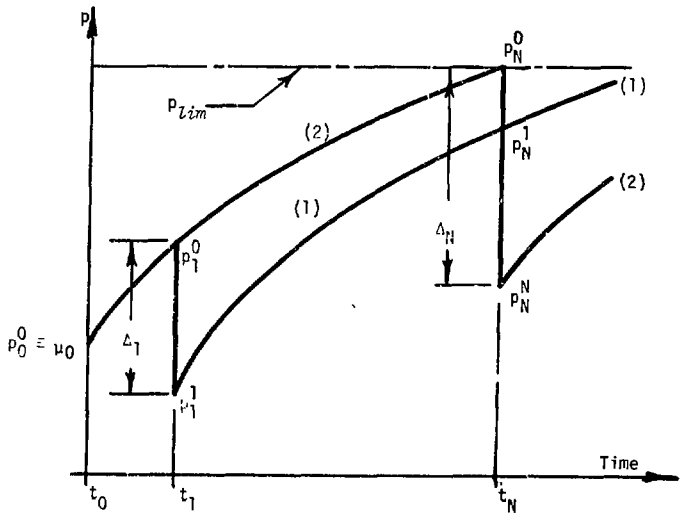


Figure 5.7. Relationships involved in scalar optimal management program.

The optimality of case (2) is verified if after both programs have included one measurement, after time t_{K+N}, the variance for case (2) is below that of case (1).

In order to prove (5.154), proceed as follows. Consider the "amount of correction" Δ to the variance p at a sample as the difference between the predicted and corrected values at the sample time. From Figure 5.7, then, define

$$\Delta_1 \equiv \left(p_1^0 - p_1^1\right), \tag{5.155}$$

$$\Delta_N \equiv \left(p_N^0 - p_N^N\right). \tag{5.156}$$

It will be shown in what follows that if p_K^0 is a monotonically increasing function of t_K, then

$$\left(p_N^0 > p_1^0\right) \Rightarrow \left(\Delta_N > \Delta_1\right). \tag{5.157}$$

Then, predict Δ_1 ahead in time to t_N to show

$$\left(\Delta_N > \Delta_1\right) \Rightarrow \left(p_N^1 > p_N^N\right) \tag{5.158}$$

which proves (5.154). Finally, it is necessary to show that if sampling at t_N is superior to sampling at t_1, then for all times t_{N+R} after t_N,

$$\left(p_N^1 > p_N^N\right) \Rightarrow \left(p_{N+R}^1 > p_{N+R}^N\right). \tag{5.159}$$

First, consider the evolution of p_{K+N}^K after a measurement at time t_K:

$$p_{K+N}^K = (\phi^2)^N p_K^K + \sum_{n=1}^{N} (\phi^2)^{n-1} \omega, \tag{5.160}$$

where, if the measurement after t_K is the first measurement,

$$p_K^K = p_K^0 \left[\frac{\nu}{p_K^0 c^2 + \nu}\right]. \tag{5.161}$$

Since $p_K^0 > 0$ and $c^2 > 0$ in (5.161),

$$p_K^K < p_K^0 , \tag{5.162}$$

that is, the variance in the estimate is (expectedly) *decreased* at a measurement. In general, the variance, or uncertainty, will grow between measurements, or at least it will under certain conditions upon the combination of p_K^K, ϕ^2 and ω in (5.160), those conditions which are of interest in the monitoring problem. Thus, restrict the study here to systems which possess monotonically increasing values of predicted variance as shown in Figure 5.7. Hence, require that

$$p_N^0 > p_1^0. \tag{5.163}$$

Next, consider the corrections in (5.155) and (5.156). To deduce the inference in (5.157), from (5.149) through (5.153), find

$$\Delta_1 = p_1^0 - p_1^0 \left[\frac{\nu}{p_1^0 c^2 + \nu} \right], \tag{5.164}$$

$$\Delta_N = p_N^0 - p_N^0 \left[\frac{\nu}{p_N^0 c^2 + \nu} \right]. \tag{5.165}$$

To find conditions under which

$$\Delta_N > \Delta_1, \tag{5.166}$$

substitute (5.164) and (5.165) into the above, cross multiply by the denominators and collect terms to obtain

$$\left[\left(p_N^0 \right)^2 p_1^0 c^2 + \left(p_N^0 \right)^2 \nu \right] > \left[\left(p_1^0 \right)^2 p_N^0 c^2 + \left(p_1^0 \right)^2 \nu \right], \tag{5.167}$$

from (5.157) and (5.167) follows

> Conclusion XVI. For the scalar case of the monitoring management problem and for problems with increasing uncertainty in the state estimate between sample times, the amount of correction made to the predicted variance in the state estimate is an increasing function of the predicted value of the variance at the time of the measurement. (C.XVI)

This concept of the comparison of the amounts of estimation error correction at different measurement times is suggested in a later section as the basis for a proof in the extension of these results to the vector case.

In order to prove (5.154), establish now the inference in (5.158). Referring to Figure 5.7 and using (5.151) and (5.152B), obtain

$$p_N^0 - p_N^1 = \left[(\phi^2)^{N-1} p_1^0 + \sum_{n=1}^{N-1} (\phi^2)^{n-1} \omega\right] - \left[(\phi^2)^{N-1} p_1^1 + \sum_{n=1}^{N-1} (\phi^2)^{n-1} \omega\right]$$

$$= (\phi^2)^{N-1} \left[p_1^0 - p_1^1\right]$$

$$\equiv \phi^{2(N-1)} \Delta_1. \tag{5.168}$$

However, for a stable system,

$$\phi^2 \leq 1, \tag{5.169}$$

$$\Rightarrow \quad \left[p_N^0 - p_N^1\right] \leq \Delta_1. \tag{5.170}$$

Thus, by construction from Figure 5.7 and (5.157), from (5.170),

$$\left[\Delta_N > \Delta_1\right] \Rightarrow \left[p_N^1 > p_N^N\right], \tag{5.171}$$

from which (5.158) follows.

Finally, to demonstrate (5.159), for case (1) in (5.148),

$$p_{N+R}^1 = (\phi^2)^R p_N^1 + \sum_{n=1}^{R} (\phi^2)^{n-1} \omega, \tag{5.172}$$

and for case (2)

$$p^{N}_{N+R} = (\phi^2)^{R} p^{N}_{N} + \sum_{n=1}^{R} (\phi^2)^{n-1} \omega, \tag{5.173}$$

from which (5.159) is obviously seen to follow regardless of the value of ϕ^2. Hence, if $p^{0}_{N} \geq p_{lim}$, some error limit, sampling at the limit is seen to be optimal at the sample time *and* optimal thereafter. Thus, in the scalar case, (2) is the best monitoring program.

Notice how no restrictions were placed upon ϕ^2, ω, or ν except that the system must be stable and ω and ν as variances must be positive. Thus, Conclusion XVI includes both the zero eigenvalue case for $\phi = 1$ and the negative eigenvalue case where $0 < \phi < 1$. Thus, it is a *general* result for scalar models where the asymptotic properties (5.18) and (5.20) of the infrequent sampling problem need not necessarily apply.

Thus, the verification of (5.157) through (5.159) prove that for a *fixed* measurement position reflected in c^2 and *fixed* instrument accuracy fixed by ν, sampling at the estimation error limit is optimal.

In the original comparisons for monitoring programs (1) and (2), the assumption was made that $c_1^2 \equiv c^2$ in (5.150) and $c_N^2 \equiv c^2$ in (5.153). The general case is now considered where the characteristics of the measurement at time t_1 in program (1) are free to differ from those at time t_N in (2), that is, $c_1^2 \neq c_N^2$.

The objective of both monitoring programs under the earlier problem definition is to provide a sampling schedule which requires the *least* overall number of samples necessary to maintain the estimation error below its limit at all times. An important observation for the *scalar* case is that, for a measurement at time t_K, maximizing the time t_{K+N} before the error limit is again reached is *strictly equivalent* to minimizing the estimation error *just after* the sample at time t_K (this may *not*

be the case in the extension to the vector problem due to the linear *combinations* of increasing/decreasing responses inherent in the $\mathrm{Tr}[\cdot]$ and $\sigma^2[.,.]$ functions; this case is considered later). Thus, the objective of sampling schedule (1) is to choose c_1^{*2} such that p_1^0 is minimized and that of sampling schedule (2) is to find that c_N^{*2} which minimizes p_N^N. The optimality of the two is then established by determining which program after time t_N results in the smaller estimation error; that is, in determining which of $p_N^1(c_1^{*2})$ and $p_N^N(c_N^{*2})$ is the smaller at time t_N.

For the *scalar* case, it can be shown that the optinal measurement positions reflected in c_1^{*2} and c_2^{*2} must be independent of the *time* each measurement is taken, independent of the value of the *variance* at the times of the measurements and they must strictly be equal to each other. To see this, compare the first line of (5.150) for a sample at time t_1 with the case for a sample at time t_N in (5.153). Examining the denominators of the two expressions leads to the observation that the optimal choice for c^{*2} in both cases must be *the same*. In order to maximize the time until the estimation error limit is next reached after each measurement, p_1^1 and p_N^N must be *minimized* at the times of those measurements. From the forms of the expressions for the corrected variances, this is achieved when the denomiators in both cases are *maximized*. Clearly this occurs at the same common value

$$c_1^{*2} = c_2^{*2} \equiv c^{*2}. \tag{5.174}$$

Thus, *for the scalar case*, the optimal measurement positions as determined by c^{*2} are seen to be independent of the value of the variance p at the times of the measurements and, which is actually the same thing, independent of time. The same is obviously true of the selection of the best instrument accuracy as reflected in the measurement error variance

ν which leads to the general result for the optimal management problem for scalar systems;

> Conclusion XVII. For the scalar case of the monitoring management problem, the optimal sampling program is to sample *only* when the estimation error criterion is at its limit. (C.XVII)

Notice that the results in Conclusions XVI and XVII are general in that no restriction has been made which would limit them to the infrequent sampling problem only. The infrequent sampling problem is obviously included under them as a special case.

5.8.2 Extension to the Vector Case — Arbitrary Sampling Program — Consider the general case with n states retained in the normal mode expansion for the model, m measurements at r stochastic disturbances for the monitoring management problem with bound on error in the state estimate. As in the scalar case, assume the process starts at time t_0, then compare the following two arbitrary monitoring programs:

(1) Predict to t_1, sample at t_1 and predict to t_N;
(2) Predict to t_N, then sample.

In the problem with bound on error in the state estimate, the optimal program will be that which has the smallest value of $\mathrm{Tr}[\underset{\sim}{P}]$ after t_N. The relevant equations are, for prediction,

$$\underset{\sim}{P}^K_{K+1} = \underset{\sim}{\Phi}\underset{\sim}{P}^K_K\underset{\sim}{\Phi}^T + \underset{\sim}{\Omega}, \qquad P^0_0 \equiv \underset{\sim}{M}_0, \tag{5.175}$$

$$\underset{\sim}{P}^K_{K+N} = \underset{\sim}{\Phi}^N\underset{\sim}{P}^K_K\underset{\sim}{\Phi}^{N^T} + \sum_{n=1}^{N} \underset{\sim}{\Phi}^{n-1}\underset{\sim}{\Omega}\underset{\sim}{\Phi}^{n-1^T} \tag{5.176}$$

and for correction,

$$\underset{\sim}{P}^{K+1}_{K+1} = \underset{\sim}{P}^K_{K+1} - \underset{\sim}{P}^K_{K+1}\underset{\sim}{C}^T\left[\underset{\sim}{C}\,\underset{\sim}{P}^K_{K+1}\underset{\sim}{C}^T + \underset{\sim}{V}\right]^{-1}\underset{\sim}{C}\,\underset{\sim}{P}^K_{K+1}. \tag{5.177}$$

Assume that the same measurement matrix $\underset{\sim}{C}$ is used in both sampling programs.

Case (1)

(A) Predict from t_0 to t_1:

$$\underset{\sim}{P}_1^0 = \underset{\sim}{\Phi}\underset{\sim}{M}_0\underset{\sim}{\Phi}^T + \underset{\sim}{\Omega}; \tag{5.178}$$

(B) Sample at t_1:

$$\underset{\sim}{P}_1^1 = \underset{\sim}{P}_1^0 - \underset{\sim}{P}_1^0\underset{\sim}{C}^T\left[\underset{\sim}{C}\underset{\sim}{P}_1^0\underset{\sim}{C}^T + \underset{\sim}{V}\right]^{-1}\underset{\sim}{C}\underset{\sim}{P}_1^0$$

$$= \left(\underset{\sim}{\Phi}\underset{\sim}{M}_0\underset{\sim}{\Phi}^T + \underset{\sim}{\Omega}\right) - \left(\underset{\sim}{\Phi}\underset{\sim}{M}_0\underset{\sim}{\Phi}^T + \underset{\sim}{\Omega}\right)\underset{\sim}{C}^T\left[\underset{\sim}{C}\left(\underset{\sim}{\Phi}\underset{\sim}{M}_0\underset{\sim}{\Phi}^T + \underset{\sim}{\Omega}\right)\underset{\sim}{C}^T + \underset{\sim}{V}\right]^{-1}\underset{\sim}{C}\left(\underset{\sim}{\Phi}\underset{\sim}{M}_0\underset{\sim}{\Phi}^T + \underset{\sim}{\Omega}\right); \tag{5.179}$$

(C) Predict to t_N: using (5.176), obtain

$$\underset{\sim}{P}_N^1 = \underset{\sim}{\Phi}^{N-1}\underset{\sim}{P}_1^1\underset{\sim}{\Phi}^{N-1^T} + \sum_{n=1}^{N-1}\underset{\sim}{\Phi}^{n-1}\underset{\sim}{\Omega}\underset{\sim}{\Phi}^{n-1^T}$$

$$= \left(\underset{\sim}{\Phi}^N\underset{\sim}{M}_0\underset{\sim}{\Phi}^{N^T} + \sum_{n=1}^{N}\underset{\sim}{\Phi}^{n-1}\underset{\sim}{\Omega}\underset{\sim}{\Phi}^{n-1^T}\right)$$

$$- \underset{\sim}{\Phi}^{N-1}\left\{\left(\underset{\sim}{\Phi}\underset{\sim}{M}_0\underset{\sim}{\Phi}^T + \underset{\sim}{\Omega}\right)\underset{\sim}{C}^T\left[\underset{\sim}{C}\left(\underset{\sim}{\Phi}\underset{\sim}{M}_0\underset{\sim}{\Phi}^T + \underset{\sim}{\Omega}\right)\underset{\sim}{C}^T + \underset{\sim}{V}\right]^{-1}\underset{\sim}{C}\left(\underset{\sim}{\Phi}\underset{\sim}{M}_0\underset{\sim}{\Phi}^T + \underset{\sim}{\Omega}\right)\right\}\underset{\sim}{\Phi}^{N-1} \tag{5.180}$$

Case (2)

(A) Predict t_N:

$$\underset{\sim}{P}_N^0 = \underset{\sim}{\Phi}^N\underset{\sim}{M}_0\underset{\sim}{\Phi}^{N^T} + \sum_{n=1}^{N}\underset{\sim}{\Phi}^{n-1}\underset{\sim}{\Omega}\underset{\sim}{\Phi}^{n-1^T}; \tag{5.181}$$

(B) Sample at t_N:

$$\underset{\sim}{P}_N^N = \underset{\sim}{P}_N^0 - \underset{\sim}{P}_N^0\underset{\sim}{C}^T\left[\underset{\sim}{C}\underset{\sim}{P}_N^0\underset{\sim}{C}^T + \underset{\sim}{V}\right]^{-1}\underset{\sim}{C}\underset{\sim}{P}_N^0$$

$$= \left(\underset{\sim}{\Phi}^N\underset{\sim}{M}_0\underset{\sim}{\Phi}^{N^T} + \sum_{n=1}^{N}\underset{\sim}{\Phi}^{n-1}\underset{\sim}{\Omega}\underset{\sim}{\Phi}^{n-1^T}\right) - \left(\underset{\sim}{\Phi}^N\underset{\sim}{M}_0\underset{\sim}{\Phi}^{N^T} + \sum_{n=1}^{N}\underset{\sim}{\Phi}^{n-1}\underset{\sim}{\Omega}\underset{\sim}{\Phi}^{n-1^T}\right)\underset{\sim}{C}^T$$

$$\times\left[\underset{\sim}{C}\left(\underset{\sim}{\Phi}^N\underset{\sim}{M}_0\underset{\sim}{\Phi}^{N^T} + \sum_{n=1}^{N}\underset{\sim}{\Phi}^{n-1}\underset{\sim}{\Omega}\underset{\sim}{\Phi}^{n-1^T}\right)\underset{\sim}{C}^T + \underset{\sim}{V}\right]^{-1}\underset{\sim}{C}\left(\underset{\sim}{\Phi}^N\underset{\sim}{M}_0\underset{\sim}{\Phi}^{N^T} + \sum_{n=1}^{N}\underset{\sim}{\Phi}^{n-1}\underset{\sim}{\Omega}\underset{\sim}{\Phi}^{n-1^T}\right) \tag{5.182}$$

In order to establish the optimality of program (2), it is required to find conditions on $\underset{\sim}{\Phi}$, $\underset{\sim}{\Omega}$, and $\underset{\sim}{M}_0$ such that

$$\mathrm{Tr}\left[\underset{\sim}{P}_N^1\right] > \mathrm{Tr}\left[\underset{\sim}{P}_N^N\right]. \tag{5.183}$$

In general, this is difficult to accomplish owing to the complexity involved in comparing traces of inverses of matrices. Since it is so difficult to say anything at the symbolic level of (5.180) and (5.182), an example with $n = 2$, $m = 1$, and $r = 1$ was developed algebraically which resulted in the same result as found with the scalar case in Conclusion XVII. However, an analytical result for the general case has not been found.

Thus, a general result for the optimal management problem for the vector case has not been obtained analytically, though the results for the scalar case do suggest extension to the vector problem. Numerical determination of the optimal sampling schedule for specific problems, though tedious, should be possible with dynamic programming (see Meier, et al. [92] for a related problem).

5.8.3 Extension to the Vector Case — Infrequent Sampling Program — Following the discussion for the scalar case where it was found that the amount of correction to the estimation error criterion was directly proportional to its predicted value at the time of a measurement, it is desired to show the following for the vector case of monitoring with a bound on error in the state estimate:

(A) Predict to time t_K, sample there and find the correction

$$\Delta \mathrm{Tr}_K \equiv \mathrm{Tr}\left[\underset{\sim}{P}_K^0 - \underset{\sim}{P}_K^K\right]; \tag{5.184A}$$

(B) Predict to time t_{K+N} then sample and find the correction

$$\Delta Tr_{K+N} \equiv Tr\left[\underset{\sim}{P}^{0}_{K+N} - \underset{\sim}{P}^{K+N}_{K+N}\right]; \tag{5.184B}$$

(C) Show that

$$\left(Tr\left[\underset{\sim}{P}^{0}_{K+N}\right] > Tr\left[\underset{\sim}{P}^{0}_{K}\right]\right) \Rightarrow \left(\Delta Tr_{K+N} > \Delta Tr_{K}\right); \tag{5.184C}$$

(D) Finally, predict the case in (A) ahead to t_{K+N} and show

$$\left(\Delta Tr_{K+N} > \Delta Tr_{K}\right) \Rightarrow \left(Tr\left[\underset{\sim}{P}^{K+N}_{K+N}\right] < Tr\left[\underset{\sim}{P}^{K}_{K+N}\right]\right). \tag{5.184D}$$

Graphically, these relationships are shown in Figure 5.8 which is simply the vector analog to Figure 5.7 for the scalar case.

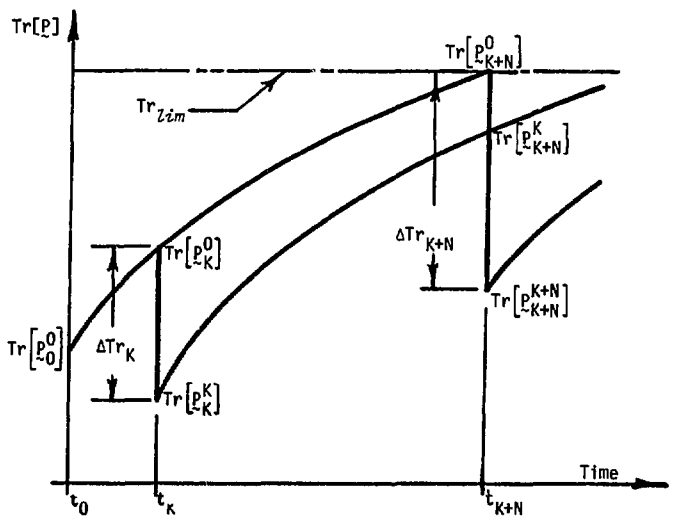


Figure 5.8. Asymptotic relationships for Tr[P] in the vector optimal management problem.

It is assumed that times t_K and t_{K+N} are sufficiently long to permit the approximations in the infrequent sampling problem (5.18) and (5.20)) to apply at each sample. With these simplifications, obtain from (5.22)

$$\mathrm{Tr}\left[\underset{\sim}{P}^0_K\right] \simeq \left[\underset{\sim}{P}^0_0\right]_{11} + K\Omega_{11} + \mathrm{Tr}\left[\underset{\sim}{\Omega}_{SS}\right], \tag{5.185}$$

$$\mathrm{Tr}\left[\underset{\sim}{P}^0_{K+N}\right] \simeq \left[\underset{\sim}{P}^0_0\right]_{11} + (K+N)\Omega_{11} + \mathrm{Tr}\left[\underset{\sim}{\Omega}_{SS}\right], \tag{5.186}$$

$$\underset{\sim}{P}^K_K = \underset{\sim}{P}^0_K - \underset{\sim}{P}^0_K\underset{\sim}{C}^T_K\left[\underset{\sim}{C}_K\underset{\sim}{P}^0_K\underset{\sim}{C}^T_K + \underset{\sim}{V}\right]^{-1}\underset{\sim}{C}_K\underset{\sim}{P}^0_K, \tag{5.187}$$

$$\underset{\sim}{P}^{K+N}_{K+N} = \underset{\sim}{P}^0_{K+N} - \underset{\sim}{P}^0_{K+N}\underset{\sim}{C}^T_{K+N}\left[\underset{\sim}{C}_{K+N}\underset{\sim}{P}^0_{K+N}\underset{\sim}{C}^T_{K+N} + \underset{\sim}{V}\right]^{-1}\underset{\sim}{C}_{K+N}\underset{\sim}{P}^0_{K+N}. \tag{5.188}$$

For consistency, as before assume that

$$\underset{\sim}{C}_K = \underset{\sim}{C}_{K+N} \equiv \underset{\sim}{C} \tag{5.189}$$

at both measurement times. Thus in (5.184A),

$$\begin{aligned}\Delta\mathrm{Tr}_K &= \mathrm{Tr}\left[\underset{\sim}{P}^0_K\right] - \mathrm{Tr}\left[\underset{\sim}{P}^0_K - \underset{\sim}{P}^0_K\underset{\sim}{C}^T\left[\underset{\sim}{C}\underset{\sim}{P}^0_K\underset{\sim}{C}^T + \underset{\sim}{V}\right]^{-1}\underset{\sim}{C}\underset{\sim}{P}^0_K\right] \\ &= \mathrm{Tr}\left[\underset{\sim}{P}^0_K\underset{\sim}{C}^T\left[\underset{\sim}{C}\underset{\sim}{P}^0_K\underset{\sim}{C}^T + \underset{\sim}{V}\right]^{-1}\underset{\sim}{C}\underset{\sim}{P}^0_K\right].\end{aligned} \tag{5.190}$$

Similarly, for (5.184B),

$$\Delta\mathrm{Tr}_{K+N} = \mathrm{Tr}\left[\underset{\sim}{P}^0_{K+N}\underset{\sim}{C}^T\left[\underset{\sim}{C}\underset{\sim}{P}^0_{K+N}\underset{\sim}{C}^T + \underset{\sim}{V}\right]^{-1}\underset{\sim}{C}\underset{\sim}{P}^0_{K+N}\right]. \tag{5.191}$$

It is required in (5.184C) to compare $\Delta\mathrm{Tr}_K$ in (5.190) with $\Delta\mathrm{Tr}_{K+N}$ in (5.191). Making substitutions for $\underset{\sim}{P}^0_K$ and $\underset{\sim}{P}^0_{K+N}$ for the matrices in (5.185) and (5.186) shows that the *only* difference in $\underset{\sim}{P}^0_K$ and $\underset{\sim}{P}^0_{K+N}$ is in the value of their (1,1)-elements; see the second terms in (5.185) and (5.186). This results from the infrequent sampling approximations.

Even with this simplification, analytical comparisons in (5.190) and (5.191) could not be found to substantiate (5.184C). Approaches used included use of the following theorem from matrix theory for the inversion of a partitioned matrix:

THEOREM If $\underset{\sim}{A}_{11}$ is nonsingular, then the inverse of the partitioned matrix

$$\underset{\sim}{A} \equiv \left[\begin{array}{c|c} \underset{\sim}{A}_{11} & \underset{\sim}{A}_{12} \\ \hline \underset{\sim}{A}_{21} & \underset{\sim}{A}_{22} \end{array}\right]$$

is given by

$$\underset{\sim}{A}^{-1} = \left[\begin{array}{c|c} \underset{\sim}{A}^{-1} + \underset{\sim}{X}\underset{\sim}{\Theta}^{-1}\underset{\sim}{Y} & -\underset{\sim}{X}\underset{\sim}{\Theta}^{-1} \\ \hline -\underset{\sim}{\Theta}^{-1}\underset{\sim}{Y} & \underset{\sim}{\Theta}^{-1} \end{array}\right],$$

where

$$\underset{\sim}{X} = \underset{\sim}{A}_{11}^{-1}\underset{\sim}{A}_{12}, \qquad \underset{\sim}{Y} = \underset{\sim}{A}_{21}\underset{\sim}{A}_{11}^{-1},$$

$$\underset{\sim}{\Theta} = \underset{\sim}{A}_{22} - \underset{\sim}{A}_{21}\underset{\sim}{X}. \tag{5.192}$$

Attempting to use (5.192) in comparing (5.190) and (5.191) where the partition is taken to have $\underset{\sim}{A}_{11}$ include only the (1,1)-elements of those matrices shows that allowing *only* the (1,1)-element of $\underset{\sim}{P}^0_K$ and $\underset{\sim}{P}^0_{K+N}$ to be different effects *every element* in the inner inverses in (5.190) and (5.191); thus, use of (5.192) does not seem to help.

It was thought that use could be made of the

MATRIX INVERSION LEMMA For $\underset{\sim}{P} > 0$ and $\underset{\sim}{V} > 0$,

$$\underset{\sim}{P} - \underset{\sim}{P}\underset{\sim}{C}^T[\underset{\sim}{C}\underset{\sim}{P}\underset{\sim}{C}^T + \underset{\sim}{V}]^{-1}\underset{\sim}{C}\underset{\sim}{P} = [\underset{\sim}{P}^{-1} + \underset{\sim}{C}^T\underset{\sim}{V}^{-1}\underset{\sim}{C}]^{-1}, \tag{5.193}$$

(see Sorensen in Leondes [78], p. 254).

However, though the number of terms in ΔTr_K and ΔTr_{K+N} decreases, the complexity in their comparison increases. Thus, the pursuit of an analytical statement for the solution of the optical management problem in the vector case was abandoned.

5.8.4 Suggestion of a Heuristic Proof for the Vector Case — For the general management problem (of which the infrequent sampling problem is only a special case), the following heuristic proof is offered in substantiation of the optimality of sampling only at the error limit when the model state is a vector.

Suppose the problem started at time t_0 and now is at time t_K. The following two sampling programs as before are to be compared:

(1) Sample at t_K and predict to t_{K+N};
(2) Predict to t_{K+N} and sample. (5.194)

For consistency, assume again that the same measurement matrix $\underset{\sim}{C}$ is used in each case. Then, the optimality of (2) over (1) can be shown by proving that, at t_{K+N},

$$\text{Tr}\left[\underset{\sim}{P}^{K+N}_{K+N}\right] \text{ for case (2)} < \text{Tr}\left[\underset{\sim}{P}^{K}_{K+N}\right] \text{ for case (1).} \qquad (5.195)$$

The above may be proven with a simple extension of the scalar results of Conclusion XVI to the vector case. This extension can be made after making the following

> Conjecture A. The absolute values of the individual elements of the predicted covariance matrix in the linear recurrence (5.175) are monotonically increasing functions of time. (C.A)

Numerical experiments have shown the above to be true but an analytical proof has not been obtained: Assume the conjecture to be true in what follows.

The optimality of case (2) can be established by reasoning as follows at the first measurement time t_K;

(1) Assume the measurement associated with the matrix $\underset{\sim}{C}$ effects *all* the modal state variables, that is, information is gained in the estimate of each state of the filter at a measurement;
(2) The information obtained in each mode decreases the absolute value of every element of the covariance matrix during a measurement;
(3) Conjecture A implies that the absolute values of all the elements of the predicted covariance matrix $[\underset{\sim}{P}^{0}_{K+N}]$ at time t_{K+N} are larger than those of $[\underset{\sim}{P}^{0}_{K}]$ at time t_K;
(4) Then, from Conclusion XVI for the scalar case, the absolute value of the correction to *each element* of $[\underset{\sim}{P}^{0}_{K+N}]$ at t_{K+N} should be greater than that to each element of $[\underset{\sim}{P}^{0}_{K}]$ at t_K;
(5) By the uniqueness of the solutions of linear recurrences, the elements of $[\underset{\sim}{P}^{K+N}_{K+N}]$ for a sample at time t_{K+N} must thus be smaller in absolute value than those of $[\underset{\sim}{P}^{K}_{K+N}]$ at t_{K+N} for a sample at t_K. (5.196)

A graphical interpretation of this even for a small number of retained modes adds more confusion than clarification to the above. Such a pictorial description would follow Figure 5.7 for the scalar case, where such a graph can now be thought to apply to *each element* of the $(n \times n)$ covariance matrix.

If the above construction has validity, it applies to both the trace of the state estimate error covariance matrix and to the variance of the system output estimate anywhere in the medium. Thus, in both the monitoring problem with bound on state estimate error and that with bound on output estimate error, the optimal management program would be to sample *only* when the error criterion reaches its limit.

Though a proof has not been found, the concepts presented here may prove to form a basis for future solution of the optimal management problem for the multidimensional case.

5.9 Extension to Systems in Noncartesian Coordinates: General Result for the Infrequent Sampling Problem

Duff and Naylor [34], in Chapter 6 on the general theory of eigenvalues and eigensystems discuss at length conditions under which partial differential equations of applied mathematics are separable. Results are given there of conditions under which eigensystems for given coordinate systems can be found. The results presented in this thesis for the infrequent sampling problem, based upon properties (5.18) and (5.20), extend directly to systems in any coordinate system for which complete orthogonal eigensystems can be found; the requirement is only that the first eigenvalue must dominate the asymptotic response, a condition which has been seen to admit a wide variety of suitable boundary conditions. As developed in Young [131], no-flow boundary conditions can be

used in conjunction with pseudo-sources at the boundaries of actual systems in the coupling of component models to one another, greatly extending the application of infrequent monitoring theory.

The results of Conclusion XIV for systems with fixed boundary conditions extend as a worst case to systems in any separable coordinate system where a complete set of orthogonal eigenfunctions may be found. In those cases, fixed boundary conditions, or emission or radiation boundary conditions lead to the modified separation property in (5.119); this results in the necessity of solving for the position of maximum variance in the output estimate in the monitoring problem with bound on output error as a function of time. This is not a serious difficulty and does boast the property that as in Conclusion XII for no-flow boundary conditions, once the position of maximum variance is found at the first sample, that position will be the position of the maximum variance for *all* subsequent samples. Thus, the time-varying maximization in (5.119) and (5.120) for one-dimensional diffusion with fixed boundary conditions, or for systems with emission or radiation boundary conditions as in Conclusion XV, need be solved *only at the first sample*, the same result applying for all other samples; the result extends directly to all systems of higher dimension in separable coordinates with complete, orthogonal eigensystems.

The more ideal results of Conclusions VII and XII for systems with no-flow boundary conditions appear to also extend to systems in arbitrary coordinate systems where, again, complete orthogonal eigensystems exist. The requirement in order for the solution of the minimax problem to be independent of time in Conclusion XI is that the eigenfunction associated with the dominant eigenvalue, in this case, the zero eigenvalue, be inde-

pendent of the spatial coordinates. Consistent with this requirement, make

> Conjecture B For diffusive systems in any coordinate system where solutions may be expressed in terms of a complete, orthogonal eigensystem, the case of no-flow boundary conditions leads to a dominant eigenvalue of zero modulus and an associated eigenfunction which is independent of the spatial coordinates. (C.B)

Examples include diffusive systems in cylindrical coordinates. For a system with a no-flow boundary condition at radius r = R, the eigenfunctions are Bessel functions; the eigenvalues are the positive roots of

$$\frac{d}{dt} J_0(\lambda R) = 0, \tag{5.197}$$

the first of which is zero. The eigenfunctions are

$$e_n(r) = J_0(\lambda_n r), \tag{5.198}$$

but since $\lambda_1 = 0$, the first eigenfunction is independent of r (see Mac Robert [62], for an extensive treatement of Bessel functions in the area of spherical harmonics).

Another example concerns radial and latitudinal atmospheric pollutant transport on a global scale (see Young [131], Chapter 4). It can be seen that eigenfunctions in the radial direction are Bessel functions while those in the latitudinal direction are the Legendre polynomials. Both eigensystems possess zero first eigenvalues and related eigenfunctions which are independent of the spatial variables.

In cases such as these, the complete separation of the minimax problem as in Conclusion X into two independent problems in minimization and maximization, *both* of which may be solved independently of time leads to an elegantly simple solution of the infrequent monitoring problem with bound on error in the output estimate.

The following general results for diffusive systems in various dimensions and coordinate systems summarize the extension of the one-dimensional results of this chapter to the general case in multiple dimensions.

> Conclusion XVIII. The complete solution of the design problem for an infrequent sampling monitor may be determined at the first sample time, the results being optimal for all subsequent sample times. The optimal sampling management program appears to be to sample *only* when the estimation error criterion is at its limit. These results apply to diffusive systems in separable coordinate systems with homogeneous boundary conditions where complete, orthogonal eigensystems exist and to normal mode models of arbitrary finite dimension.
>
> (C.XVIII)

CHAPTER 6. NUMERICAL EXPERIMENTS

Examples are presented in this chapter which serve to numerically substantiate many of the analytical results of Chapter 5. The discrete-time Kalman Filter algorithm of Chapter 4 is programmed as shown in PROGRAM KALMAN (see Appendix F) using the normal mode problem formulation of Chapter 3 and the time-discretization algorithms of Chapter 4 and Appendices A, B, and C. The first-order gradient optimization algorithm with linear constraints described in Section 5.3.6 (see Westley [127]) is coded as SUBROUTINE KEELE and included as part of KALMAN. For the case $m = 2$, for the optimal positioning of two noise-corrupted measurement devices, and for a one-dimensional diffusive medium, it is found to be convenient to generate contour plots of the value of the estimate error criterion (either $\mathrm{Tr}[P^K_{K+N}(\underset{\sim}{z}_K)]$ or $[P^K_{K+N}(\underset{\sim}{z}_K)]_{11}$) as a function of the two measurement device position coordinates $[\underset{\sim}{z}_K]_1$ and $[\underset{\sim}{z}_K]_2$, at various times t_{K+N}. The surfaces shown in these plots with the high level of information they contain were instrumental in arriving at many of the conclusions of Chapter 5.

The basic problem to be considered is developed in the following section; various examples based upon it to demonstrate the more salient features of the infrequent monitoring problem are included in subsequent sections.

6.1 Problems in One-Dimensional Diffusion with No-Flow Boundary Conditions: Method of Solution

Consider a one-dimensional problem in diffusion including scavenging described as follows:

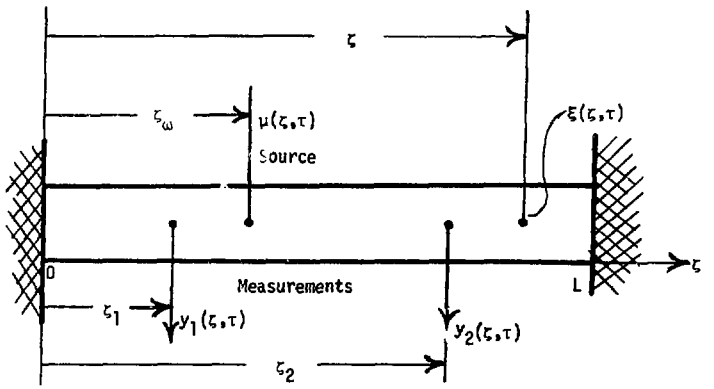


Figure 6.1. One-dimensional Diffusive system example.

For the pollutant concentration $\xi(\zeta,\tau)$, consider the following initial-boundary value problem:

$$\frac{\partial \xi}{\partial \tau} = K \frac{\partial^2 \xi}{\partial \zeta^2} - \gamma \xi + \mu(\zeta,\tau); \tag{6.1}$$

$$\frac{\partial \xi(\zeta,\tau)}{\partial \zeta} = 0, \qquad \zeta = 0, \qquad \zeta = L; \tag{6.2}$$

$$\xi(\zeta,0) = \sum_{n=1}^{n} \cos\left((n-1)\frac{\pi}{L}\zeta\right). \tag{6.3}$$

The single stochastic point source is defined by

$$\mu(\zeta,\tau) = \omega(\tau)\delta(\zeta - \zeta_\omega),$$

$$E[\omega(\tau)] = 0$$

$$E[\omega(\tau_1)\omega(\tau_2)] = W\delta(\tau_1 - \tau_2). \tag{6.4}$$

In the interest of generality, transform the problem to dimensionless functions of time and space as follows:

$$z \equiv \frac{\zeta}{L};$$

$$t \equiv \frac{K\tau}{L^2};$$

$$\alpha \equiv \frac{L^2\gamma}{K};$$

$$w \equiv \frac{L^2\omega}{K}. \tag{6.5}$$

Substitution of (6.5) into (6.1) yields the following dimensionless form for the one-dimensional diffusion initial-boundary value problem:

$$\frac{\partial\xi}{\partial t} = \frac{\partial^2\xi}{\partial z^2} - \alpha\xi + f(z,t); \tag{6.6}$$

$$\frac{\partial\xi(z,t)}{\partial z} = 0, \qquad z = 0, \qquad z = 1; \tag{6.7}$$

$$\xi(z,0) = \sum_{n=1}^{n} \cos\left((n - 1)\,\pi z\right); \tag{6.8}$$

and where the dimensionless point source is given by

$$f(z,t) = w(t)\delta(z - z_w),$$

$$E[w(t)] = 0,$$

$$E[w(t_1)w(t_2)] = W\delta(t_1 - t_2). \tag{6.9}$$

With these generalizations, the modal resistances, capacitances and eigenvalues from Table (3.31) become the following for the dimensionless problem with scavenging:

	R_n	C_n	λ_n
$n = 1$	∞	1	α
$n = 2,3,\ldots$	$\frac{2}{(n-1)^2\pi^2}$	$\frac{1}{2}$	$\left((n-1)^2\pi^2 + \alpha\right)$

(6.10)

The forcing terms from (3.35) become

$$\left[\frac{1}{C_n}\cos\left((n-1)\pi z_w\right)\right]w(t), \qquad n = 1,2,\ldots \tag{6.11}$$

The pollutant concentration at any point z from (3.35) becomes

$$\xi(z,t) = \sum_{n=1}^{\infty} x_n(t)\cos\left((n-1)\pi z\right). \tag{6.12}$$

For a sufficient number of modes to be both theoretically interesting and computationally expedient, choose $n = 5$ for the number of terms retained in the expansion in (6.12). This choice will be studied later as to its effect upon the outcome of the infrequent sampling problem.

Thus, the modal state equations may be written in dimensionless variables as follows:

$$\underline{\dot{x}} = \underline{A}\,\underline{x} + \underline{D}\,\underline{w}$$

$$\begin{bmatrix}\dot{x}_1\\ \dot{x}_2\\ \dot{x}_3\\ \dot{x}_4\\ \dot{x}_5\end{bmatrix} = \begin{bmatrix}-\alpha & & & & \\ & -(\pi^2+\alpha) & & & \\ & & -(4\pi^2+\alpha) & & \\ & & & -(9\pi^2+\alpha) & \\ & & & & -(16\pi^2+\alpha)\end{bmatrix}\begin{bmatrix}x_1\\ x_2\\ x_3\\ x_4\\ x_5\end{bmatrix} + \begin{bmatrix}1\\ 2\cos(\pi z_w)\\ 2\cos(2\pi z_w)\\ 2\cos(3\pi z_w)\\ 2\cos(4\pi z_w)\end{bmatrix} w(t). \tag{6.13}$$

The initial pollutant distribution $\xi(z,0)$ is chosen as in (6.8) so that, from (3.33), the initial modal state variables are written simply as

$$\underset{\sim}{x}(0) \equiv \underset{\sim}{m}_0 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \tag{6.14}$$

The covariance of the error in the estimate in the initial state is chosen to be

$$P_0^0 \equiv \underset{\sim}{M}_0 = \begin{bmatrix} 0.05 & & & & \bigcirc \\ & 0.01 & & & \\ & & 0.00001 & & \\ & & & 0.00001 & \\ \bigcirc & & & & 0.00001 \end{bmatrix}. \tag{6.15}$$

For $m \equiv 2$, the two noise-corrupted measurements in the vector $\underset{\sim}{y}$ are given by

$$\begin{matrix} \underset{\sim}{y} & = & & \underset{\sim}{C} & & \underset{\sim}{x} & + & \underset{\sim}{v} \end{matrix}$$

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} 1 & \cos(\pi z_1) & \cos(2\pi z_1) \ldots \\ 1 & \cos(\pi z_2) & \cos(2\pi z_2) \ldots \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{bmatrix} + \begin{bmatrix} v_1(t) \\ v_2(t) \end{bmatrix}, \tag{6.16}$$

where the mean value of the measurement noise

$$E[\underset{\sim}{v}] \equiv \underset{\sim}{0}. \tag{6.17}$$

Choose the position of the stochastic source as

$$z_w \equiv 0.3. \tag{6.18}$$

For this case, scavenging is ignored so that

$$\alpha \equiv 0.0. \tag{6.19}$$

Let the source and measurement noise statistics be defined by the following covariance matrices:

$$W \equiv 0.125, \tag{6.20}$$

$$\underset{\sim}{V} \equiv \begin{bmatrix} 0.050 & 0 \\ 0 & 0.025 \end{bmatrix}; \tag{6.21}$$

A typical output record of the problem description from KALMAN is shown in Figuure 6.2. The data corresponds to a problem with a bound on the error in the state estimate where the error limit $Tr_{lim} \equiv 0.075$. At each measurement time, NSEARCH ≡ 5 random starting vectors are to be used in the measurement position optimizations. The initial guess for the measurement positions is chosen as $\underset{\sim}{z}_K \equiv [0.15,0.15]^T$ (called Z). The computed values for $\underset{\sim}{A}$ and $\underset{\sim}{D}$ are shown. For a stepsize of DT ≡ 0.01, the so-called Paynter number = 35, that is, the number of terms used in the series approximation for $e^{\underset{\sim}{A}T}$ in (4.9), for an error criterion of EPS = 0.00001. The state transition matrix $\underset{\sim}{\Phi}^K_{K+1}$ (called AK) and the discrete disturbance distribution matrix $\underset{\sim}{\Gamma}^K_{K+1}$ (called DK) from (4.12) are computed along with the incremental disturbance noise covariance matrix $\underset{\sim}{\Omega}_{K+1}$ from (4.14) and Appendix B (called WKP1). The steady-state disturbance covariance matrix $\underset{SS}{\underset{\sim}{\Omega}}$ from (5.19) and (5.20) (*including* the term $\left[\underset{SS}{\underset{\sim}{\Omega}}\right]_{11}$) is listed as WSS along with the number of timesteps NSS necessary for the infrequent sampling approximations to be valid; see (5.78) for the value $\epsilon \equiv$ 100*EPS (same EPS given above).

For the monitoring problem with bound on error in the state estimate, a measurement is necessary whenever at time t_{K+N}, $Tr[\underset{\sim}{P}^K_{K+N}(\underset{\sim}{z}^*_K)] \geq Tr_{lim}$. At each sample, an attempt is made to locate the global optimum of the measurement position vector $\underset{\sim}{z}^*_{K+N}$ such that

$$P^*_{11} = \min_{\underset{\sim}{z}_{K+N}} \left[\underset{\sim}{P}^{K+N}_{K+N}(\underset{\sim}{z}_{K+N})\right]_{11}. \tag{6.22}$$

For the initial guess of $\underset{\sim}{z}_{K+N} \equiv [0.15,0.15]^T$, and for NSEARCH ≡ 5 other random starting vectors, the constrained first-order gradient algorithm

```
DISCRETE KALMAN FILTER SIMULATION PROGRAM, VER5/2/75 , RUN NO.  1

PROBLEM INPUT IS AS FOLLOWS...

        N          L          M          LL          NTL ------IPLT ------IOUT      LENGTH
        5          2          2           1            2  1 1 0 0 1 0000000000      40000

       TO         T1         DT        NOPD         EPS        KMAX
    .0E+00  1.000E+00  1.000E-02          0  1.000E-05         100

EXAMPLE TO SHOW GROWTH OF TRACE[P(K,K+N)] SURFACE WITH TIME T(K+N).
ITS SHAPE APPROACHES THAT OF [P(K,K)]11 SURFACE ASYMPTOTICALLY FOR LARGE N.

MO      VECTOR IS...

 1.000E+00  1.000E+00  1.000E+00  1.000E+00  1.000E+00

CAPMO   MATRIX IS...

 5.000E-02    -.0E+00    -.0E+00    -.0E+00    -.0E+00
   -.0E+00  1.000E-02    -.0E+00    -.0E+00    -.0E+00
   -.0E+00    -.0E+00  1.000E-05    -.0E+00    -.0E+00
   -.0E+00    -.0E+00    -.0E+00  1.000E-05    -.0E+00
   -.0E+00    -.0E+00    -.0E+00    -.0E+00  1.000E-05

CAPW    MATRIX IS...

 1.250E-01

CAPV    MATRIX IS...

 5.000E-02    -.0E+00
   -.0E+00  2.500E-02

ZW      VECTOR IS...

 3.000E-01

Z       VECTOR IS...

 1.500E-01  1.500E-01

NUMBER OF POINTS FOR RANDOM SEARCH INITIALIZATION (NSEARCH) =     5


THIS IS A MONITORING PROBLEM OF THE FIRST KIND
WITH A CONSTRAINT ON THE ALLOWABLE ERROR IN THE STATE ESTIMATE
THE ESTIMATION ERROR CRITERION IS THE TRACE[P(K,K+N)]
THE CONSTRAINT ON THE ERROR IN THE STATE ESTIMATE IS FIXED AT

TRLIM = 7.500E-02
```

Figure 6.2A. Problem description from PROGRAM KALMAN.

```
PARAMETERS FOR SYSTEM DESCRIPTION ARE...

DIFFUSION CONSTANT   K =  1.000E+00
LENGTH OF MEDIUM     L =  1.000E+00
SCAVENGING RATE ALPHA =      .0E+00

A       MATRIX IS...

    -.0E+00      .0E+00      .0E+00      .0E+00      .0E+00
     .0E+00 -9.870E+00      .0E+00      .0E+00      .0E+00
     .0E+00      .0E+00 -3.948E+01      .0E+00      .0E+00
     .0E+00      .0E+00      .0E+00 -8.883E+01      .0E+00
     .0E+00      .0E+00      .0E+00      .0E+00 -1.578E+02

D       MATRIX IS...

 1.000E+00
 1.176E+00
-6.180E-01
-1.902E+00
-1.618E+00

THE PAYNTER NUMBER K =    25 FOR EPS =  1.000E-05 AND DELTAT =  1.000E-02
THE MATRICES WHICH FOLLOW ARE THE DISCRETE-TIME STATE, CONTROL AND NOISE TRANSITION MATRICES.

AK      MATRIX IS...

 1.000E+00      .0E+00      .0E+00      .0E+00      .0E+00
     .0E+00 9.060E-01      .0E+00      .0E+00      .0E+00
     .0E+00      .0E+00 6.738E-01      .0E+00      .0E+00
     .0E+00      .0E+00      .0E+00 4.114E-01      .0E+00
     .0E+00      .0E+00      .0E+00      .0E+00 2.062E-01

DK      MATRIX IS...

 1.000E-02
 1.119E-02
-5.106E-03
-1.260E-02
-8.134E-03

WKP1    MATRIX IS...

 1.250E-03  1.399E-03 -6.383E-04 -1.576E-03 -1.017E-03
 1.399E-03  1.568E-03 -7.168E-04 -1.776E-03 -1.152E-03
-6.383E-04 -7.168E-04  3.301E-04  8.278E-04  5.453E-04
-1.576E-03 -1.776E-03  8.278E-04  2.115E-03  1.427E-03
-1.017E-03 -1.152E-03  5.453E-04  1.427E-03  9.921E-04

WSS     MATRIX IS...

 9.000E-02  1.438E-02 -1.957E-03 -2.677E-03 -1.281E-03
 1.438E-02  8.751E-03 -1.840E-03 -2.832E-03 -1.417E-03
-1.957E-03 -1.840E-03  6.047E-04  1.145E-03  6.333E-04
-2.677E-03 -2.012E-03  1.145E-03  2.154E-03  1.559E-03
-1.281E-03 -1.417E-03  6.333E-04  1.559E-03  1.036E-03

THE NUMBER OF TERMS IN THE TRUNCATED MATRIX CONVOLUTION SERIES
FOR THE STEADY-STATE VALUE OF (WSS) NSS =  71
```

Figure 6.2B. Problem description from PROGRAM KALMAN.

KEELE produced the results for the first measurement partially shown in Figure 6.3. The global minimum is chosen as the best minimum found after the NSEARCH + 1 attempts.

Figure 6.4 is a time history of $\mathrm{Tr}[P^K_{K+N}(\underset{\sim}{z}^*_K)]$, that is, a plot of the performance criterion with the optimal measurement positions from time t_K used in its evaluation between measurement times t_K and t_{K+N}. Three sample times are shown at t = 0.09, 0.48, and 0.88. At each sample, the optimal positions of the m = 2 measurement devices with covariances given in (6.21) are found such that the time to the next sample is maximized. Examples of actual state and optimal state estimates are shown in Figure 6.5. In the plots, those labeled X(·) are plots of states with time, those labeled XH(·), (mnemonic for $\hat{x}$ or x-hat) are the corresponding state estimates.

In assessing the global optimality of $\underset{\sim}{z}^*_K$ and P^*_{11} found at time t_K (as in (6.22)), contour plots are constructed for the objective function $[P^K_K(\underset{\sim}{z}_K)]_{11}$ plotted against $[\underset{\sim}{z}_K]_1$ horizontally and $[\underset{\sim}{z}_K]_2$ vertically. The minimum plotted value is noted with a "*", the maximum with a "ø". In between are nineteen equally spaced levels, denoted with the symbols (*)( )(1)( )(2)( )...(9)( )(ø). The actual evolution of the optimization calculations can be followed with such contour plots in order to understand the procedures of the algorithm. More importantly, study of the contours serves as an important method of understanding the nature of the design problem, since the plots convey a level of information otherwise not available through tabular listings or other means.

At each sample time, say t_{K+N}, the predicted covariance matrix P^K_{K+N} is written out for post processing and after the entire time interval in the monitoring problem is covered, contour plots of the

```
          N          M          NE         IEXP       NLIN       FMAX       IW
          2          4           0          0          50        500        1

0    CONVG      DELT     EPSLON     RHO      DELTAP     TOL
  1.000E-05 1.000E-07 1.000E-07 1.000E-07 1.000E-07 1.000E-10


THE NUMBER OF CALLS TO FVAL IS    1
   1.30934685E-02  1.00000000E+00  2.13471279E-01
THE NUMBER OF CALLS TO FVAL IS    7
   1.27494646E-02  1.00000000E+00  1.63265064E-01

ITERATION NO.   1
FNUM   FUNCTION VALUE             Z(1)...

THE NUMBER OF CALLS TO FVAL IS    1
   1.36764440E-02  4.37071939E-01  6.01669468E-01
THE NUMBER OF CALLS TO FVAL IS   19
   1.26441469E-02  2.11255890E-01  5.15546271E-01

ITERATION NO.   2
FNUM   FUNCTION VALUE             Z(1)...

THE NUMBER OF CALLS TO FVAL IS    1
   1.46922084E-02  3.74187011E-01  8.92581636E-01
THE NUMBER OF CALLS TO FVAL IS   16
   1.26441469E-02  2.11254872E-01  5.15547999E-01

ITERATION NO.   3
FNUM   FUNCTION VALUE             Z(1)...

THE NUMBER OF CALLS TO FVAL IS    1
   1.62042943E-02  5.07662490E-01  8.00551916E-01
THE NUMBER OF CALLS TO FVAL IS   19
   1.26441469E-02  2.11262648E-01  5.15552953E-01

ITERATION NO.   4
FNUM   FUNCTION VALUE             Z(1)...

THE NUMBER OF CALLS TO FVAL IS    1
   1.56617995E-02  3.88314891E-01  2.78840503E-01
THE NUMBER OF CALLS TO FVAL IS   11
   1.26962670E-02  6.62177265E-01  1.67144930E-01

ITERATION NO.   5
FNUM   FUNCTION VALUE             Z(1)...

THE NUMBER OF CALLS TO FVAL IS    1
   1.32010582E-02  2.27311246E-01  6.63829703E-01
THE NUMBER OF CALLS TO FVAL IS  442
   1.26441469E-02  2.11255964E-01  5.15548379E-01

BEST LOCAL MINIMUM FOUND AFTER   6 TRYS IS...
       1.26441469E-02  2.11254872E-01  5.15547999E-01
```

Figure 6.3. Summary of results of minimization of $\left[P_{\underset{\sim}{K}}^{K}(\underset{\sim}{z}_K)\right]_{11}$ at the first sample time from SUBROUTINE KEELE.

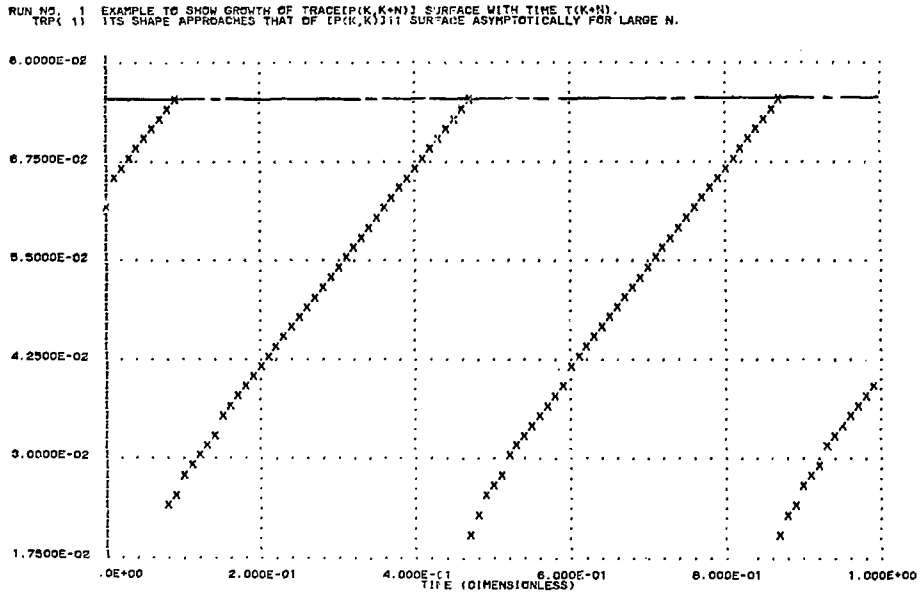


Figure 6.4. Time response of $\mathrm{Tr}\left[P_{K+N}^{K}\left(z_K^*\right)\right]$, the performance criterion for the optimal monitoring problem with bound on error in the state estimate; samples occur at t_K = 0.09, 0.48, and 0.88.

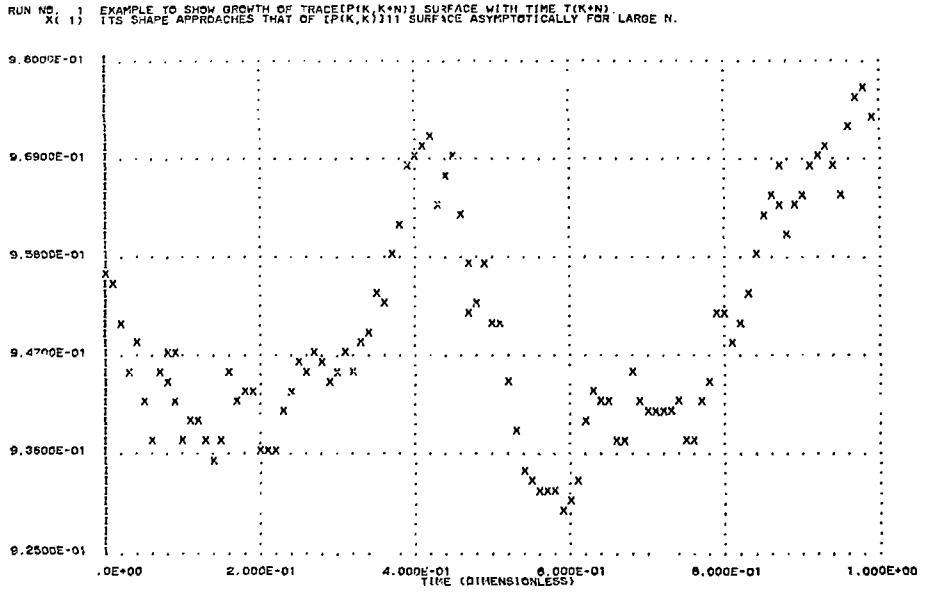


Figure 6.5A. Trajectory of the first modal state, $\left[x_{K+N}\right]_1$, versus time t_{K+N}.

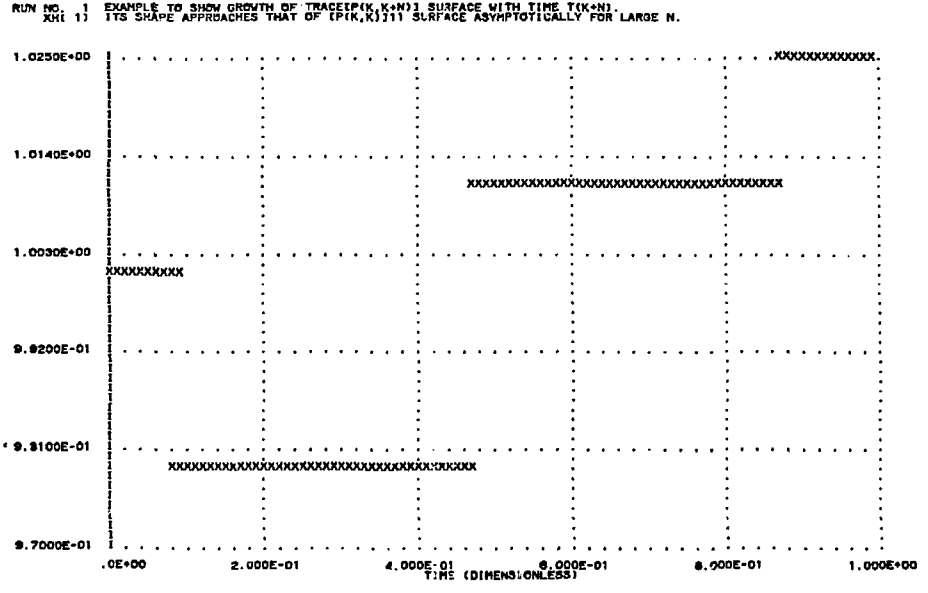


Figure 6.5B. Trajectory of the optimal estimate of the first modal state, $\left[\hat{\underline{x}}_{K+N}^{K}\right]_1$, versus time t_{K+N}.

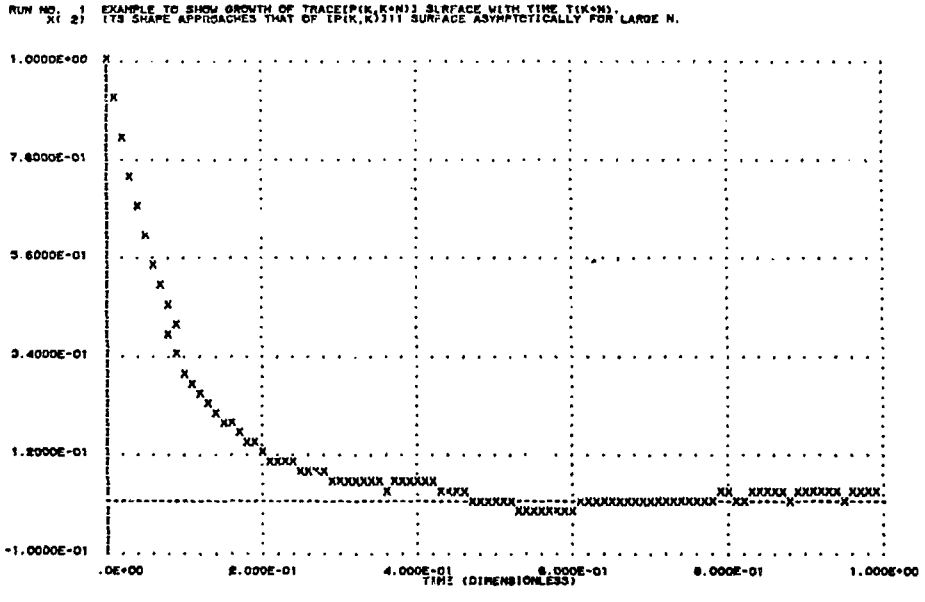


Figure 6.5C. Trajectory of the second modal state, $\left[x_{K+N}\right]_2$, versus time t_{K+N}.

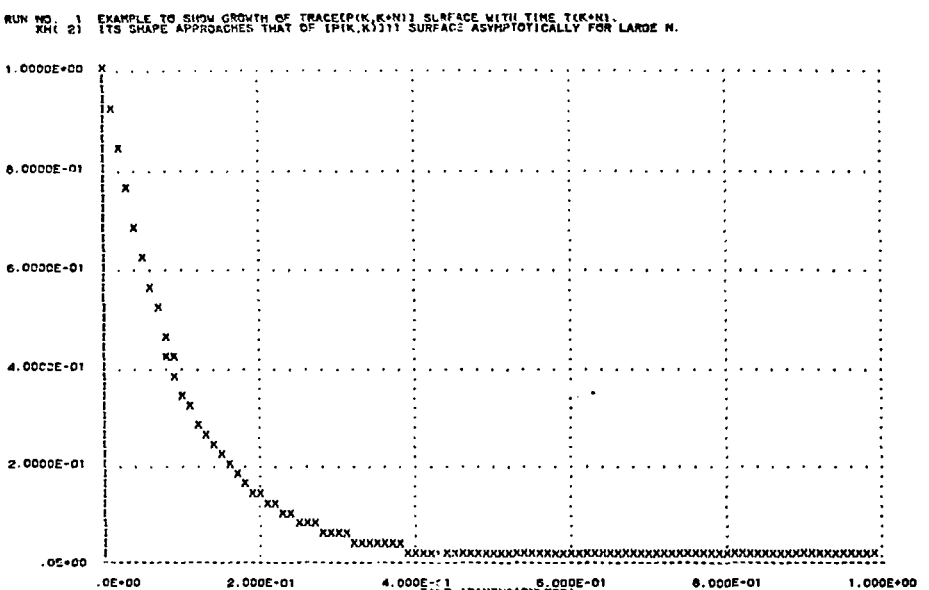


Figure 6.5D. Trajectory of the optimal estimate of the second modal state, $\left[\hat{\underset{\sim}{x}}^{K}_{K+N}\right]_2$, versus time t_{K+N}.

$[\underset{\sim}{P}^{K+N}_{K+N}(\underset{\sim}{z}_{K+N})]_{11}$ surfaces are made for each sample time. Much use of these plots is made in what follows.

6.2 Problems with Bound on State Estimation Error

6.2.1 Asymptotic Response of State Estimation Error — For the monitoring problem with bound on allowable error in the estimate of the modal state vector, it is necessary to make a measurement whenever for a time t_{K+N},

$$\mathrm{Tr}\left[\underset{\sim}{P}^{K}_{K+N}(\underset{\sim}{z}_{K})\right] \geq \mathrm{Tr}_{lim}, \tag{6.23}$$

that is, whenever the trace of the error covariance matrix predicted from the last measurement at positions $\underset{\sim}{z}_K$ at time t_K to time t_{K+N} reaches the estimation error limit Tr_{lim}.

In order to numerically substantiate the fundamental results for the infrequent sampling problem contained in conclusions II, III, and IIIA, the relationship between $\mathrm{Tr}[\underset{\sim}{P}^{K}_{K+N}(\underset{\sim}{z}_{K})]$ and $[\underset{\sim}{P}^{K}_{K}(\underset{\sim}{z}_{K})]_{11}$ is now considered. Suppose the monitoring problem is started at time t_0 with $\underset{\sim}{P}^{0}_{0} \equiv \underset{\sim}{M}_0$ as the initial value of the error covariance matrix; let its value then be predicted ahead to time t_K when

$$\mathrm{Tr}\left[\underset{\sim}{P}^{0}_{K}\right] = \mathrm{Tr}\left[\underset{\sim}{\Phi}^{K}\underset{\sim}{M}_0\underset{\sim}{\Phi}^{K^T} + \sum_{n=1}^{K}\underset{\sim}{\Phi}^{n-1}\underset{\sim}{\Omega}\underset{\sim}{\Phi}^{n-1^T}\right] \geq \mathrm{Tr}_{lim}, \tag{6.24}$$

at which point a measurement must be made. The monitoring design problem is to choose $\underset{\sim}{z}^{*}_{K}$ at time t_K so that the maximum time t_{K+N} results when

$$\mathrm{Tr}\left[\underset{\sim}{P}^{K}_{K+N}(\underset{\sim}{z}_{K})\right] \geq \mathrm{Tr}_{lim}, \tag{6.25}$$

For a measurement at $\underset{\sim}{z}_K$, the corrected estimation error covariance matrix immediately after the measurement is given by

$$\underline{P}_K^K(\underline{z}_K) = \underline{P}_K^0 - \underline{P}_K^0\underline{C}(\underline{z}_K)^T\left[\underline{C}(\underline{z}_K)\underline{P}_K^0\underline{C}(\underline{z}_K)^T + \underline{V}\right]^{-1}\underline{C}(\underline{z}_K)\underline{P}_K^0, \qquad (6.26)$$

where

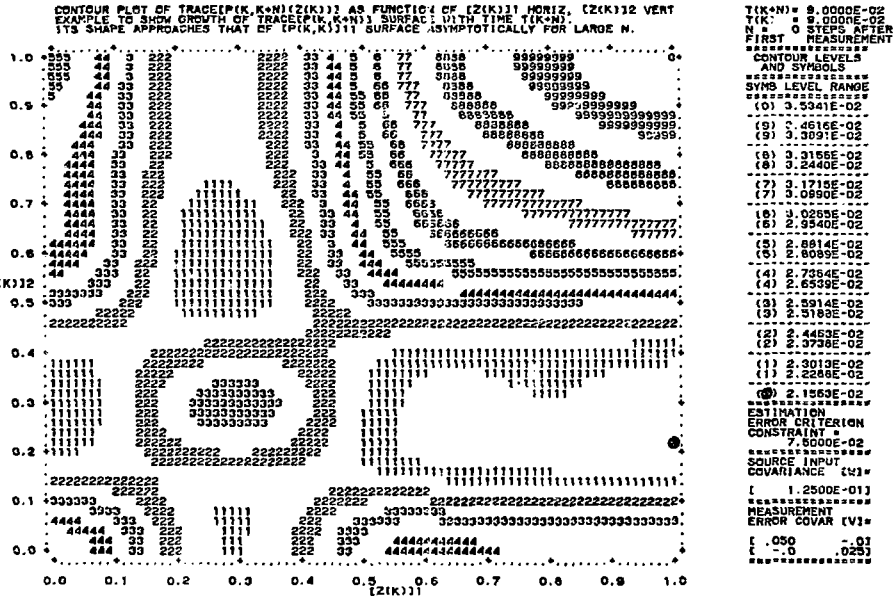
$$\underline{C}(\underline{z}_K) \equiv \begin{bmatrix} 1 & \cos(\pi z_1) & \cos(2\pi z_1) \ldots \\ 1 & \cos(\pi z_2) & \cos(2\pi z_2) \ldots \end{bmatrix}. \qquad (6.27)$$

In order to generate a contour plot of $\mathrm{Tr}[\underline{P}_K^K(\underline{z}_K)]$ from (6.26), plot values of $\mathrm{Tr}[\underline{P}_K^K(\underline{z}_K)]$ for all values of the elements of $\underline{z}_K$ over the full length of the medium ($0 \le z_1 \le 1$ and $0 \le z_2 \le 1$ in (6.27)). The surface for the first sample at $t_K = 0.09$ is shown in Figure 6.6.

To study the evolution of the trace of the predicted error covariance with time as a function of the measurements at time t_K, let

$$\begin{aligned}
\underline{P}_{K+1}^K(\underline{z}_K) &= \underline{\Phi}\underline{P}_K^K(\underline{z}_K)\underline{\Phi}^T + \underline{\Omega}; \\
\underline{P}_{K+2}^K(\underline{z}_K) &= \underline{\Phi}\underline{P}_{K+1}^K(\underline{z}_K)\underline{\Phi}^T + \underline{\Omega} \\
&= \underline{\Phi}^2\underline{P}_K^K(\underline{z}_K)\underline{\Phi}^{2T} + \underline{\Phi}\underline{\Omega}\underline{\Phi}^T + \underline{\Omega}; \\
&\;\;\vdots \qquad\qquad \vdots \qquad\qquad \vdots \\
\underline{P}_{K+N}^K(\underline{z}_K) &= \underline{\Phi}^N\underline{P}_K^K(\underline{z}_K)\underline{\Phi}^{NT} + \sum_{n=1}^{N}\underline{\Phi}^{n-1}\underline{\Omega}\underline{\Phi}^{n-1T}.
\end{aligned} \qquad (6.28)$$

Contours of the traces of the above predicted covariance matrices at times t_{K+1}, t_{K+5}, t_{K+10}, t_{K+11}, and t_{K+15} as functions of $\underline{z}_K$ are shown in Figure 6.7. Notice how the global minimum "*" moves with time. Note also how the error in the estimate in the region near the stochastic source ($z_w = 0.3$ along both coordinates z_1 and z_2) increases in value as time grows relative to the rest of the surface due to greater uncertainty in the estimate in that area.



T(K+N)= 9.0000E-02
T(K) = 9.0000E-02
N = 0 STEPS AFTER
FIRST MEASUREMENT

CONTOUR LEVELS AND SYMBOLS

SYMB	LEVEL RANGE
(0)	3.5341E-02
(9)	3.4616E-02
(9)	3.3891E-02
(8)	3.3166E-02
(8)	3.2440E-02
(7)	3.1715E-02
(7)	3.0990E-02
(6)	3.0265E-02
(6)	2.9540E-02
(5)	2.8814E-02
(5)	2.8089E-02
(4)	2.7364E-02
(4)	2.6639E-02
(3)	2.5914E-02
(3)	2.5189E-02
(2)	2.4463E-02
(2)	2.3738E-02
(1)	2.3013E-02
(1)	2.2288E-02
(@)	2.1563E-02

ESTIMATION ERROR CRITERION CONSTRAINT = 7.5000E-02

SOURCE INPUT COVARIANCE [V]=

[1.2500E-01]

MEASUREMENT ERROR COVAR [V]=

[.050 -.01
[-.0 .025]

Figure 6.6. Contour plot of $\mathrm{Tr}\left[P_K^K(z_K)\right]$ at first measurement time, $t_K = 0.09$.

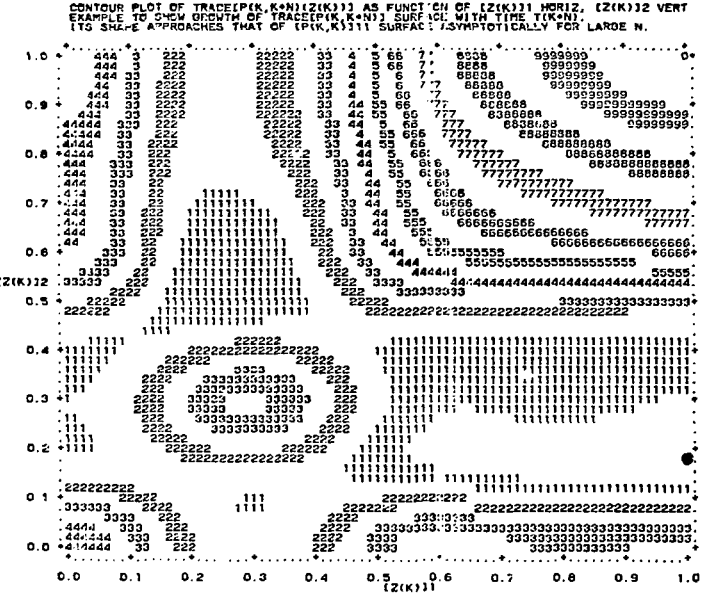


Figure 6.7A. Contour plot of $\mathrm{Tr}\left[P^{K}_{K+1|K}(z_K)\right]$ at time t_{K+1} = 0.10, one timestep after first measurement.

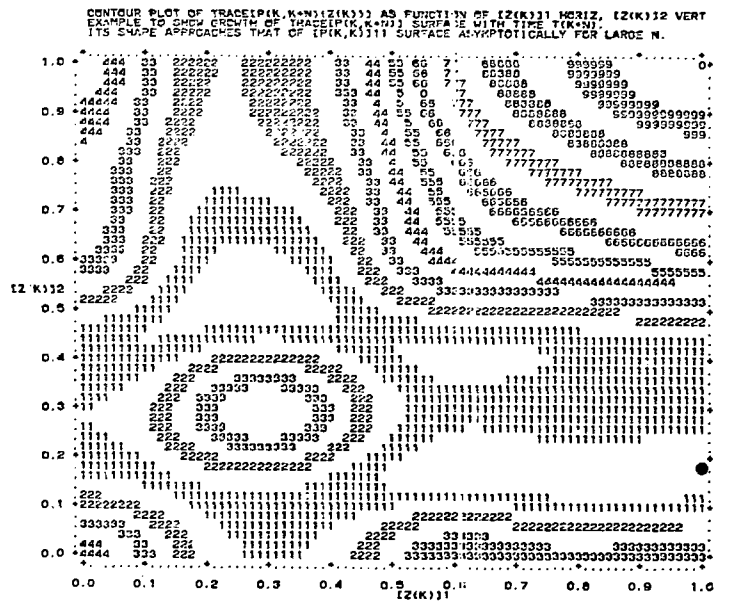


Figure 6.7B. Contour plot of $\mathrm{Tr}\left[P^{K}_{K+5}\left(z_K\right)\right]$ at time t_{K+5} = 0.14, five timesteps after first measurement.

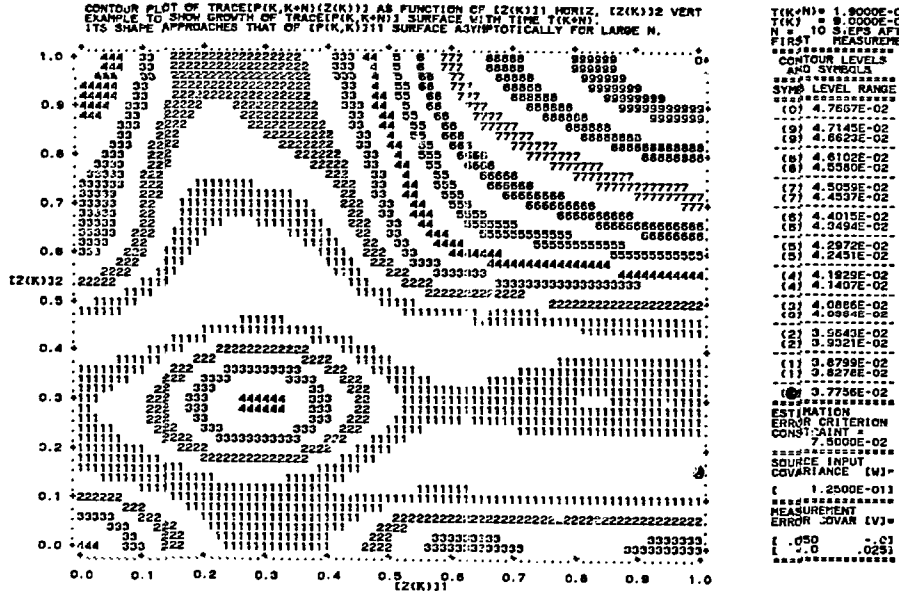


Figure 8.7C. Contour plot of $\mathrm{Tr}\left[P^{K}_{K+10}(z_K)\right]$ at time t_{K+10} = 0.19, ten timesteps after first measurement.

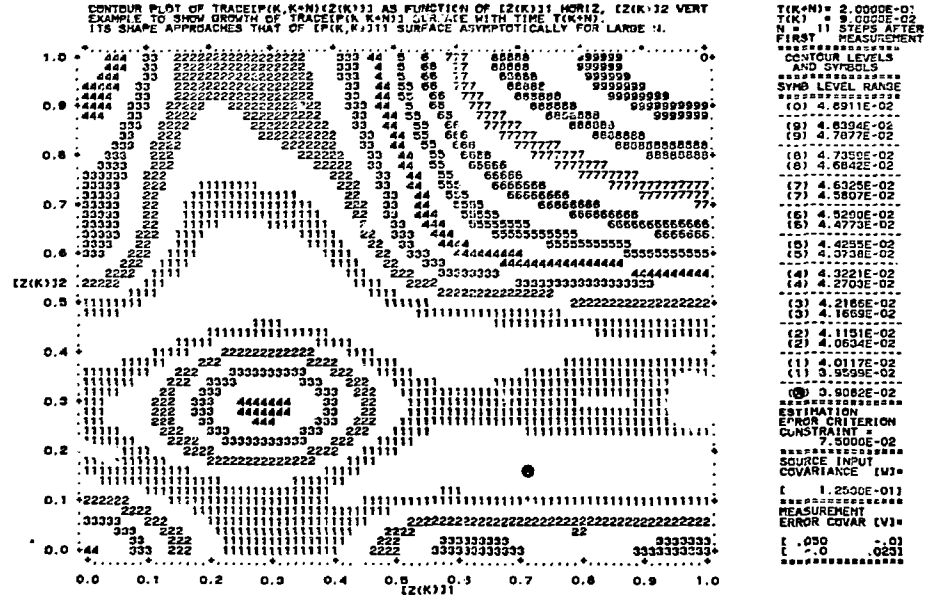


Figure 6.7D. Contour plot of $\mathrm{Tr}\left[P^{K}_{K+1|1}(z_K)\right]$ at time $t_{K+1|1}$ = 0.20, eleven timesteps after first measurement.

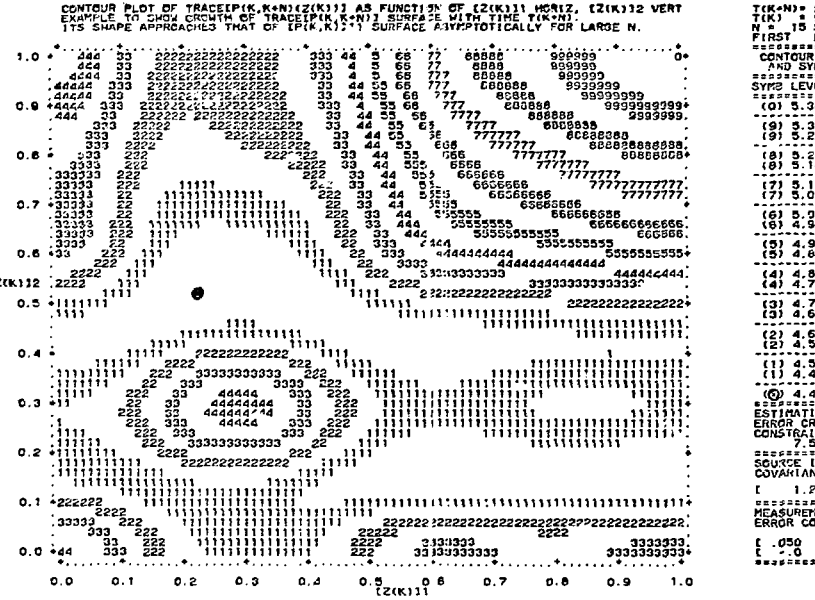


Figure 6.7E. Contour plot of $\mathrm{Tr}\left[P^{K}_{K+15}(\xi_K)\right]$ at time $t_{K+15} = 0.24$, fifteen timesteps after first measurement.

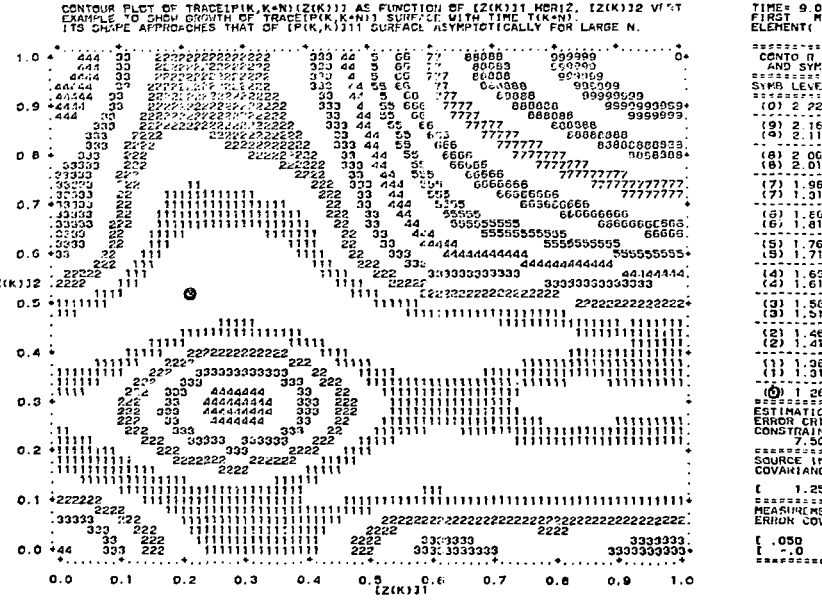


Figure 6.8. Contour plot of $\left[P^{K}_{K}(z_K)\right]_{11}$ at first measurement time, $t_K = 0.09$; compare with asymptotic response of $\mathrm{Tr}\left[P^{K}_{K+N}(z_K)\right]$ surface at $t_{K+15} = 0.24$ in Figure 6.7E.

Finally, to demonstrate the result in Conclusion II, a *contour plot* of $[\underset{\sim}{P}^K_K(\underset{\sim}{z}_K)]_{11}$ is shown in Figure 6.8. Comparing the *trace* of $\underset{\sim}{P}$ at time t_{K+15} in Figure 6.7E with the (1,1)-*element* of $\underset{\sim}{P}$ at time t_K in Figure 6.8 shows that for all values of $\underset{\sim}{z}_K$,

$$\mathrm{Tr}\left[\underset{\sim}{P}^K_{K+15}(\underset{\sim}{z}_K)\right] \simeq \left[\underset{\sim}{P}^K_K(\underset{\sim}{z}_K)\right]_{11}. \tag{6.29}$$

As N increases, so does the convergence to the result

$$\lim_{N\to\infty} \mathrm{Tr}\left[\underset{\sim}{P}^K_{K+N}(\underset{\sim}{z}_K)\right] = \left[\underset{\sim}{P}^K_K(\underset{\sim}{z}_K)\right]_{11}. \tag{6.30}$$

Another way of seeing these relationships is as follows. Write the trace of both sides of (6.28) as follows:

$$\begin{aligned}\mathrm{Tr}\left[\underset{\sim}{P}^K_{K+N}(\underset{\sim}{z}_K)\right] = &\left(\left[\underset{\sim}{P}^K_K(\underset{\sim}{z}_K)\right]_{11} + \phi_{22}^{2N}\left[\underset{\sim}{P}^K_K(\underset{\sim}{z}_K)\right]_{22} + \phi_{33}^{2N}\left[\underset{\sim}{P}^K_K(\underset{\sim}{z}_K)\right]_{33} + \cdots\right) \\ &+ \left(N[\underset{\sim}{\Omega}]_{11} + [\underset{\sim}{\Omega}]_{22}\sum_{n=1}^{N}\phi_{22}^{2(n-1)} + [\underset{\sim}{\Omega}]_{33}\sum_{n=1}^{N}\phi_{33}^{2(n-1)} + \cdots\right),\end{aligned} \tag{6.31}$$

where the two lines in (6.31) correspond with the two terms in (6.28). As N becomes large since $0 < \phi_{ii} < 1$, $i = 2,3,\ldots,n$, all the terms in the top line vanish except the first, which remains unchanged with N. For large N, the first term in the second line grows continuously at a rate $[\underset{\sim}{\Omega}]_{11}$ per time step while, according to the asymptotic relationship (5.20), all the other terms approach steady-state constants over N. The meanings of Conclusions I and II are clear in (6.31) in that at time $t_{K+\cdot}$, the *only* term of $\mathrm{Tr}[\underset{\sim}{P}^K_{K+N}(\underset{\sim}{z}_K)]$ which is still a function of $\underset{\sim}{z}_K$ is $[\underset{\sim}{P}^K_K(\underset{\sim}{z}_K)]_{11}$; *none* of the other terms effect the optimization over values of $\underset{\sim}{z}_K$.

Heuristically, the response of the surface of $\mathrm{Tr}[\underset{\sim}{P}^K_{K+N}(\underset{\sim}{z}_K)]$ over all values of $\underset{\sim}{z}_K$ as t_{K+N} grows can be thought of as follows:

$$\mathrm{Tr}\left[P^{K}_{K+N}(\underset{\sim}{z}_K)\right] = \mathrm{Tr}\left[\underset{SS}{\Omega}\right] + \left[P^{K}_{K}(\underset{\sim}{z}_K)\right]_{11} + N[\Omega]_{11} \tag{6.32}$$

which may be studied schematically as in Figure 6.9. For successive values of N, the contour of the surface of $\mathrm{Tr}[P^{K}_{K+N}(\underset{\sim}{z}_K)]$ over $\underset{\sim}{z}_K$ is composed of the contour of $[P^{K}_{K}(\underset{\sim}{z}_K)]_{11}$ plus a constant value of $\mathrm{Tr}[\underset{SS}{\Omega}]$ plus a value which grows with time, $N[\Omega]_{11}$. The *shape* of the contour $\mathrm{Tr}[P^{K}_{K+N}(\underset{\sim}{z}_K)]$ should be *exactly* the same as the shape of the $[P^{K}_{K}(\underset{\sim}{z}_K)]_{11}$ surface and the *value* of a point anywhere on those two contours should differ only by a constant.

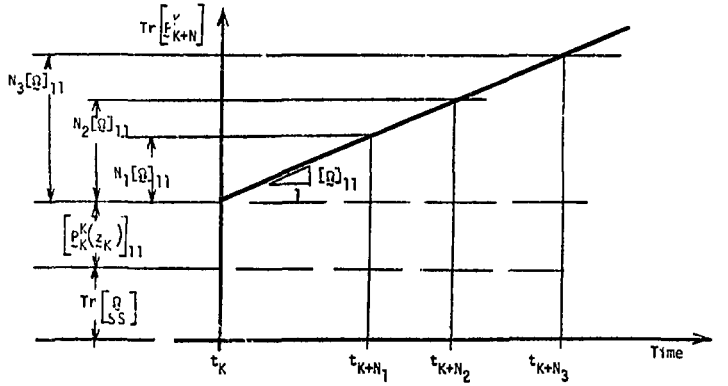


Figure 6.9. Asymptotic growth of $\mathrm{Tr}[P^{K}_{K+N}]$.

As a simple verification, compare the values on the two surfaces for the global minimum itself, the point plotted with a "*". From the calculations, for time $t_K = 0.09$,

$$\left[P^{K}_{K}(\underset{\sim}{z}^{*}_{K})\right]_{11} \doteq 0.012645. \tag{6.33}$$

For fifteen steps after the sample at $t_{K+15} = 0.24$, from Figure 6.7E,

$$\mathrm{Tr}\left[P^K_{K+15}(z^*_K)\right] = 0.044224. \tag{6.34}$$

To estimate the steady-state constant in (6.32) and Figure 6.9, hand calculate the series in (6.31) by using only the first few terms and use values for $\underset{\sim}{\Omega}$ (called WKP1) from Figure 6.2 to obtain

$\phi_{11} = 1$		$N\phi_{11} = 15.$	$\Omega_{11} = 0.001250$	$N\Omega_{11}$	$\doteq 0.01875$
$\phi_{22} = 0.9060$	$\left(1 + \phi_{22}^2 + \phi_{22}^4 + \ldots\right) \doteq 5.5485$		$\Omega_{22} = 0.001568$	$\Omega_{22}\Sigma\phi_{22}$	$\doteq 0.00870$
$\phi_{33} = 0.6738$	$\left(1 + \phi_{33}^2 + \phi_{33}^4 + \ldots\right) \doteq 1.8212$		$\Omega_{33} = 0.000330$	$\Omega_{33}\Sigma\phi_{33}$	$\doteq 0.00060$
$\phi_{44} = 0.4114$	$\left(1 + \phi_{44}^2 + \phi_{44}^4 + \ldots\right) \doteq 1.2037$		$\Omega_{44} = 0.002115$	$\Omega_{44}\Sigma\phi_{44}$	$\doteq 0.00255$
$\phi_{55} = 0.2062$	$\left(1 + \phi_{55}^2 + \phi_{55}^4 + \ldots\right) \doteq 1.0440$		$\Omega_{55} = 0.000992$	$\Omega_{55}\Sigma\phi_{55}$	$\doteq 0.00104$

$$\Rightarrow \quad N\Omega_{11} + \mathrm{Tr}\left[\underset{SS}{\Omega}\right] = N\Omega_{11} + \Omega_{22}\sum_{n=1} \phi_{22}^{2(n-1)} + \ldots \doteq 0.03163. \tag{6.35}$$

$$\Rightarrow \quad \mathrm{Tr}\left[\underset{SS}{\Omega}\right] \doteq 0.01288. \tag{6.36}$$

Thus, from (6.33) and (6.35), approximate (6.32) at z^*_K as

$$\left[P^K_K(z^*_K)\right]_{11} + N\Omega_{11} + \mathrm{Tr}\left[\underset{SS}{\Omega}\right] \doteq 0.04428. \tag{6.37}$$

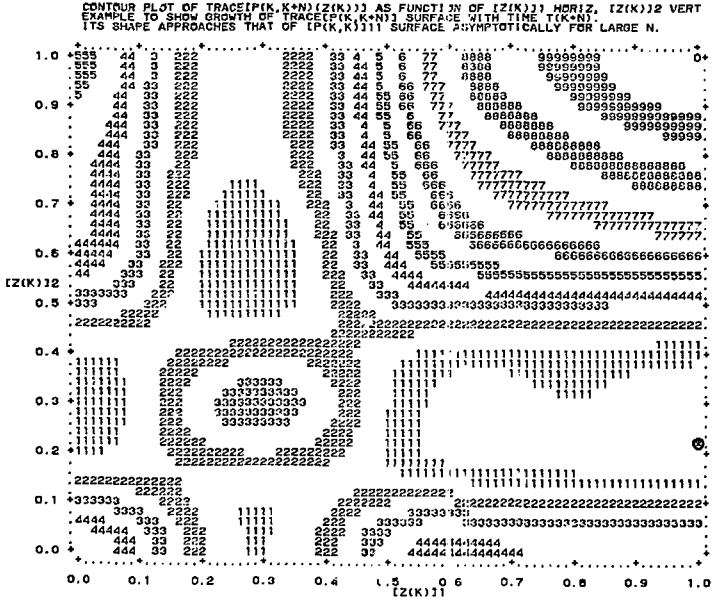
It is thus seen from a simple hand calculation that (6.34) and (6.37) are in close agreement; thus values on the two surfaces $[P^K_K(z_K)]_{11}$ and $\mathrm{Tr}[P^K_{K+15}(z_K)]$ do in fact differ only by a constant, the constant in (6.35). For increasing values of N, t_{K+N_1}, t_{K+N_2}, etc., as in Figure 6.9, for N large, any point on the $\mathrm{Tr}[P^K_{K+N}(z_K)]$ contours would then simply consist of $\mathrm{Tr}[\underset{SS}{\Omega}]$ from (6.36) added to $N[\Omega]_{11}$ plus the value at the same point on the surface of $[P^K_K(z_K)]_{11}$. The $\mathrm{Tr}[P^K_{K+N}(z_K)]$ surface is just a translation in time of the $[P^K_K(z_K)]_{11}$ surface for N large.

Another way of interpreting the asymptotic growth of the trace surface to that of the (1,1)-element of P^K_K as N becomes large is as follows.

At the time of the first sample, for $t_K = 0.09$, decompose the surface for $\mathrm{Tr}[\underset{\sim}{P}^K_K(\underset{\sim}{z}_K)]$ into surfaces for each element of the trace, that is, $[\underset{\sim}{P}^K_K(\underset{\sim}{z}_K)]_{11}$, $[\underset{\sim}{P}^K_K(\underset{\sim}{z}_K)]_{22}$, ..., $[\underset{\sim}{P}^K_K(\underset{\sim}{z}_K)]_{55}$, as shown in contour plots of Figure 6.10. The full trace, as in Figure 6.6, is shown in Figure 6.10A with the individual elements shown on succeeding plots. As time t_{K+N} becomes large, the formula for the trace in (6.31) may be rearranged as follows:

$$\begin{aligned}
\mathrm{Tr}\left[\underset{\sim}{P}^K_{K+N}\right] = {} & \left[\underset{\sim}{P}^K_K\left(\underset{\sim}{z}_K\right)\right]_{11} + [\underset{\sim}{\Omega}]_{11}N \\
& + \phi_{22}^{2N}\left[\underset{\sim}{P}^K_K\left(\underset{\sim}{z}_K\right)\right]_{22} + [\underset{\sim}{\Omega}]_{22}\sum_{n=1}^{N}\phi_{22}^{2(n-1)} \\
& \quad \vdots \qquad\qquad \vdots \\
& + \phi_{55}^{2N}\left[\underset{\sim}{P}^K_K\left(\underset{\sim}{z}_K\right)\right]_{55} + [\underset{\sim}{\Omega}]_{55}\sum_{n=1}^{N}\phi_{55}^{2(n-1)}.
\end{aligned} \tag{6.38}$$

Each line in (6.38) represents what happens to each diagonal element of $\underset{\sim}{P}^K_{K+N}$ comprising the trace as time goes on. Since $0 < \phi_{ii} < 1$, $i = 2,3,4,5$, as N becomes large, all the terms except the first loose their functional relationship with the positions of the measurement device given in $\underset{\sim}{z}_K$. In terms of the plots for $[\underset{\sim}{P}^K_{K+N}]_{22}$ through $[\underset{\sim}{P}^K_{K+N}]_{55}$ in Figures 6.10B through 6.10F, as time goes on these surfaces become flat with constant values equal to the steady-state values of the right-hand terms in (6.38). Thus, for large time, the surface $\mathrm{Tr}[\underset{\sim}{P}^K_{K+N}(\underset{\sim}{z}_K)]$ is made up of a number of steady-state "slices," a flat surface growing at the rate $[\underset{\sim}{\Omega}]_{11}$ per time step and the surface $[\underset{\sim}{P}^K_K(\underset{\sim}{z}_K)]_{11}$.



TIME= 9.0000E-02
FIRST MEASUREMENT

CONTOUR LEVELS AND SYMBOLS

SYMB	LEVEL RANGE
(0)	3.5941E-02
(9)	3.4616E-02
(9)	3.3891E-02
(8)	3.3166E-02
(8)	3.2440E-02
(7)	3.1715E-02
(7)	3.0990E-02
(6)	3.0265E-02
(6)	2.9540E-02
(5)	2.8814E-02
(5)	2.8089E-02
(4)	2.7364E-02
(4)	2.6639E-02
(3)	2.5914E-02
(3)	2.5188E-02
(2)	2.4463E-02
(2)	2.3738E-02
(1)	2.3013E-02
(1)	2.2288E-02
(0)	2.1563E-02

ESTIMATION ERROR CRITERION CONSTRAINT = 7.5000E-02

SOURCE INPUT COVARIANCE [W]=

[1.2500E-01]

MEASUREMENT ERROR COVAR [V]=

[.050 -.01]
[-.0 .025]

Figure 6.10A. Contour plot of $\mathrm{Tr}\left[P_K^{K}(z_K)\right]$ at first measurement time, $t_K = 0.09$.

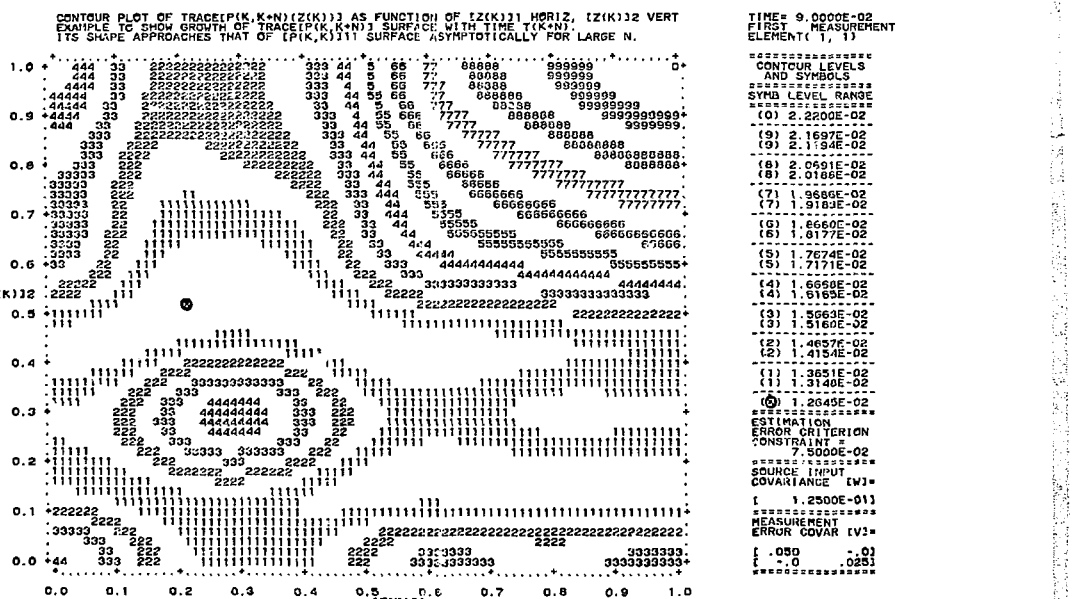


Figure 6.10B. Contour plot of first term of $\mathrm{Tr}\left[\underline{P}_K^K\ (\underline{z}_K)\right]$, $\left[\underline{P}_K^K(\underline{z}_K)\right]_{11}$.

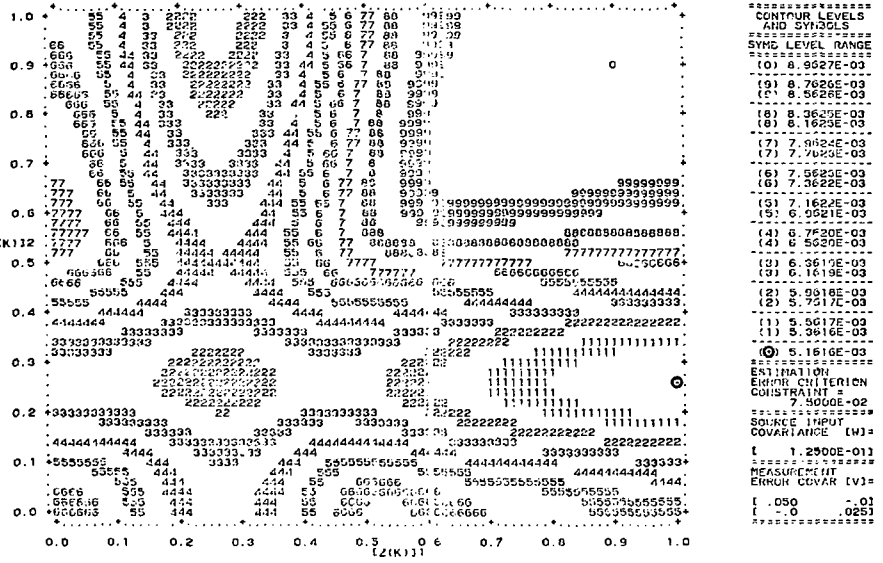


Figure 6.10C. Contour plot of second term of $\mathrm{Tr}\left[\underline{P}_K^K(z_K)\right]$, $\left[\underline{P}_K^K(z_K)\right]_{22}$.

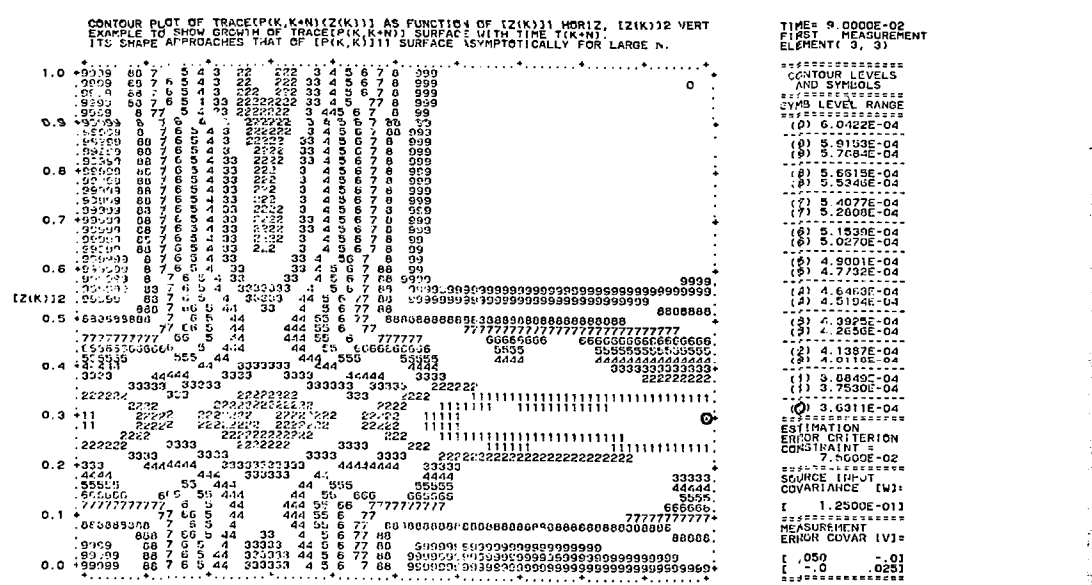


Figure 6.10D. Contour plot of third term of $\mathrm{Tr}\left[P_K^K\ (z_K)\right]$, $\left[P_K^K(z_K)\right]_{33}$

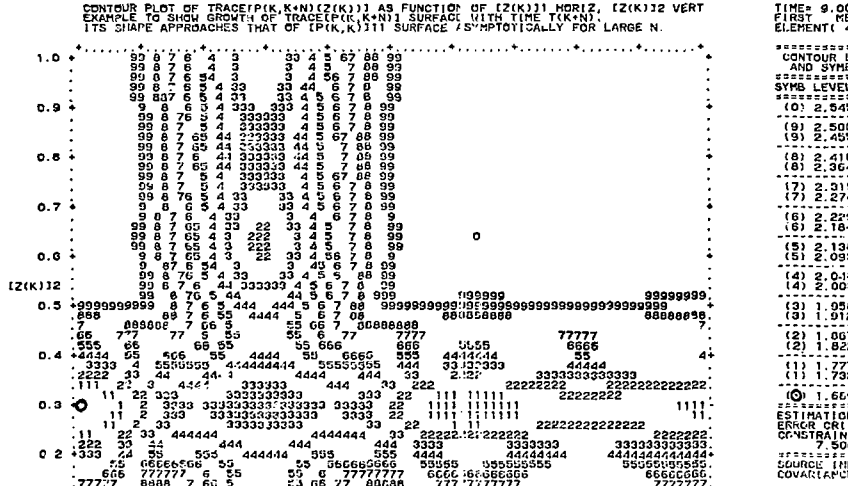


Figure 6.10E. Contour plot of fourth term of $\mathrm{Tr}\left[P_K^K\left(z_K\right), \left[P_K^K(z_K)\right]_{44}\right.$.

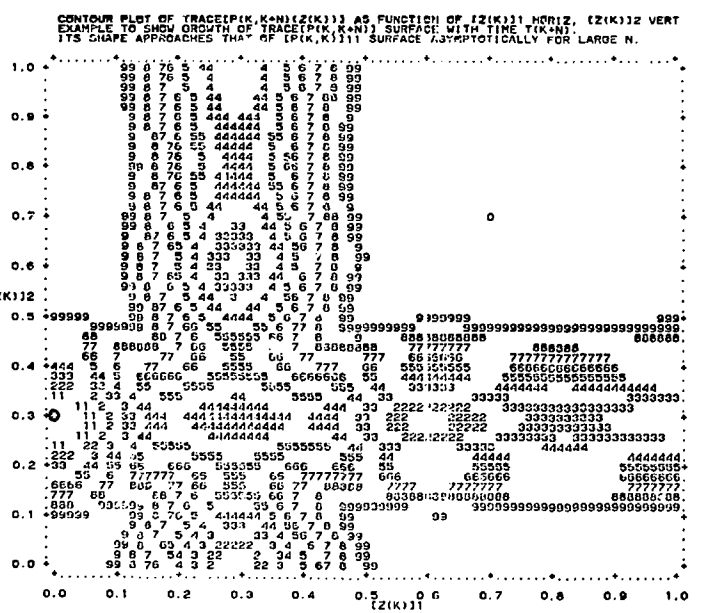


Figure 6.10F. Contour plot of fifth term of $\mathrm{Tr}\left[P_K^K\left(\underline{z}_K\right)\right]$, $\left[P_K^K\left(\underline{z}_K\right)\right]_{55}$.

6.2.2 Optimality of Measurement Locations — In Figure 6.4 was shown the trajectory $\mathrm{Tr}[\underset{\sim}{P}^{K}_{K+N}(\underset{\sim}{z}_K)]$ where the optimal choice of measurement positions was used at each measurement time. In contrast, suppose the designer felt that an intuitively good choice for the measurement positions would be to place the two statistically independent sensors right at the position of the source, that is $z_1 = z_2 = z_w = 0.3$. Figure 6.11 compares the optimal trajectory $\mathrm{Tr}[\underset{\sim}{P}^{K}_{K+N}(\underset{\sim}{z}^{*}_K)]$ of Figure 6.4 using $\min_{\underset{\sim}{z}_K} [\underset{\sim}{P}^{K}_{K}(\underset{\sim}{z}_K)]_{11}$ as the criterion at each measurement with the case with $\underset{\sim}{z}_K = [0.3,0.3]^T$, that is, with measurements positioned at the source. The optimal case is plotted with the symbol "1", that with measurements at the source with the symbol "2". Clearly, Case (1) is optimal since over a larger time interval it would result in fewer measurements necessary to maintain the estimation error below its bound.

6.2.3 Comparison of Performance Criteria — Moore [95] suggests that the minimization of the trace $\mathrm{Tr}[\underset{\sim}{P}^{K}_{K}(\underset{\sim}{z}_K)]$ at a sample time t_K may not be the best thing to do to lead to the fewest number of samples necessary over some time interval. To demonstrate that this is in fact a true conjecture, consider a slight modification to the problem of Section 6.1. Let

$$\underset{\sim}{P}^{0}_{0} \equiv \begin{bmatrix} 0.04 & & & \\ & 0.04 & & \\ & & 0.02 & \\ & & & 0.00001 \\ & & & & 0.00001 \end{bmatrix}, \tag{6.39}$$

$$\mathrm{Tr}_{lim} \equiv 0.1010, \tag{6.40}$$

and

$$T \equiv \left(t_{K+1} - t_K\right) = 0.001. \tag{6.41}$$

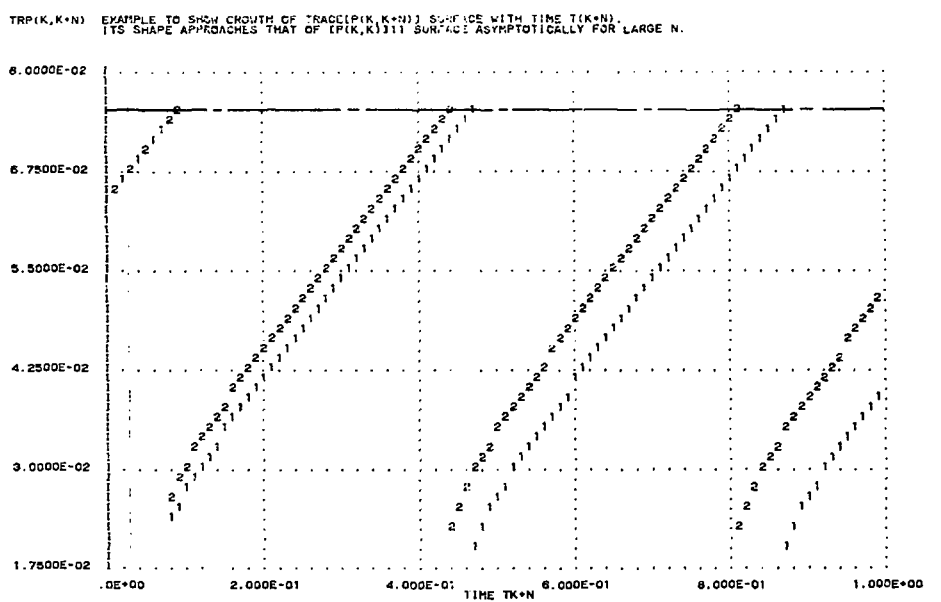


Figure 6.11. Time response of $\mathrm{Tr}\left[P^{K}_{K+N}\left(z^{*}_{K}\right)\right]$ for (1) z^{*}_{K} the result of the minimization $\min_{z_K}\left[P^{K}_{K}\left(z_K\right)\right]_{11}$ plotted with symbol "1" and (2) $\left[z^{*}_{K}\right]_1 = \left[z^{*}_{K}\right]_2 = z_w$, both measurements at the source location, plotted with symbol "2".

The other problem parameters are as before.

To measurement strategies are contrasted. The first is, at each measurement time t_K, finding $\underset{1}{z}_K^*$ such that

$$P_{11}^* = \min_{z_K} \left[\underset{\sim}{P}_K^K(z_K) \right]_{11}, \tag{6.42}$$

as before. The second is finding $\underset{2}{z}_K^*$ such that

$$Tr^* = \min_{z_K} Tr\left[\underset{\sim}{P}_K^K(z_K) \right]. \tag{6.43}$$

In this problem, measurements are necessary at t_0, the initial time and it is found that immediately after the first measurements, strategy *number 2* using $\underset{2}{z}_0^*$ appears superior to that using $\underset{1}{z}_0^*$. The two trajectories are plotted with symbols "1" and "2" in Figure 6.12. However, it is seen that at $t \cong 0.021$, the two curves cross afterwhich Criterion 1 remains superior, leading to a second measurement at $t = 0.078$ vs $t = 0.071$ for Criterion 2. At the end of the interval $0 \leq t \leq 0.1$, Criterion 1 clearly possesses the lower estimation error. Thus, it is *not* optimal to minimize the trace of the estimation error covariance matrix *at the time of the sample* but it *is* optimal to minimize its value *for large time* N, which, by Conclusion II, is equivalent to minimizing the (1,1)-element of the covariance matrix *at the time of the measurement*.

6.2.4 Effect of Instrument Accuracy — To study the effect of the quality of the measurement instruments upon the evolution of the $Tr[\underset{\sim}{P}_{K+N}^K(z_K)]$ contours in the above problem, consider the measurement error covariance matrix

$$\underset{\sim}{V} \equiv \begin{bmatrix} 0.05 & 0 \\ 0 & 0.01 \end{bmatrix} \tag{6.44}$$

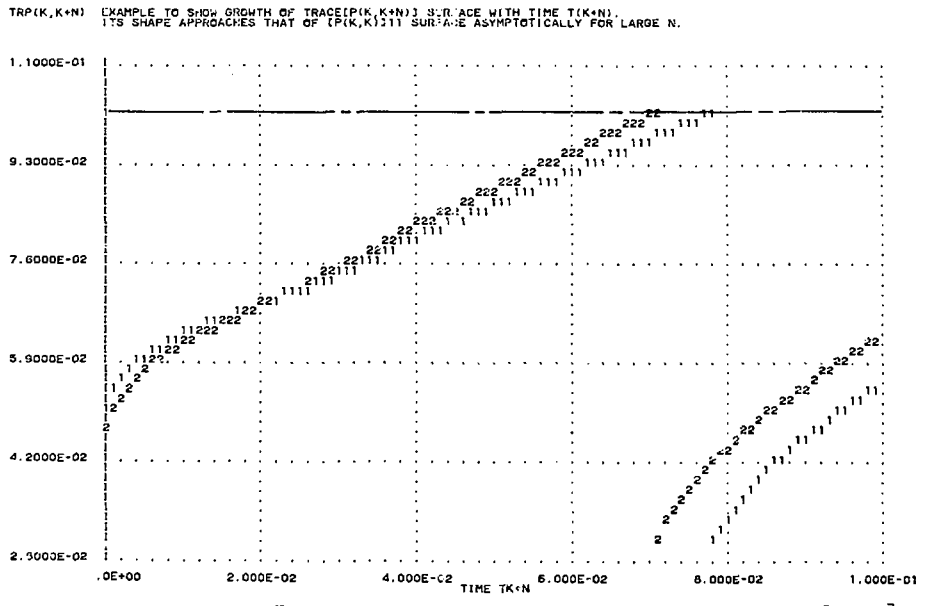


Figure 6.12. Time response of $\mathrm{Tr}\left[P^{K}_{K+N}\left(\underset{\sim}{z}^{*}_{K}\right)\right]$ for (1) $\underset{\sim}{z}^{*}_{K}$ the result of the minimization $\min_{\underset{\sim}{z}_K}\left[P^{K}_{K}\left(\underset{\sim}{z}_K\right)\right]_{11}$ plotted with symbol "1" and (2) $\underset{\sim}{z}^{*}_{K}$ the result of the minimization $\min_{\underset{\sim}{z}_K}\mathrm{Tr}\left[P^{K}_{K}\left(\underset{\sim}{z}_K\right)\right]$ plotted with symbol "2"; note how after the first measurement at t_K=0.0, (2) possesses lower estimation error but with time, the curves cross such that (1) is superior at the end of the time interval shown and thereafter.

This accounts for a 5:1 difference in variances in the two sampling devices in contrast to the 2:1 difference in the problem above. The evolution of $\mathrm{Tr}[\underset{\sim}{P}^K_{K+N}]$ is shown in Figure 6.13. The contour plot of $\mathrm{Tr}[\underset{\sim}{P}^K_K(\underset{\sim}{z}_K)]$ at $t_K = 0.09$ is shown in Figure 6.14. Contour plots of $\mathrm{Tr}[\underset{\sim}{P}^K_{K+N}(\underset{\sim}{z}_K)]$ are shown for t_{K+1}, t_{K+5}, t_{K+10}, and t_{K+15} in Figure 6.15 and finally that for $[\underset{\sim}{P}^K_K(\underset{\sim}{z}_K)]_{11}$ in Figure 6.16. In this case, since the two measurements are of much different quality than those in the previous case, the error contour is much less symmetric, showing where the more accurate sensor $[\underset{\sim}{z}]_2$ is preferred over the more inaccurate $[\underset{\sim}{z}]_1$. Notice the large motion that the global minimum "*" can make over time in a particular problem; the positions of $\underset{\sim}{z}^*_K$ the global minima can change greatly as a function of t_{K+N} for the surfaces $\mathrm{Tr}[\underset{\sim}{P}^K_{K+N}(\underset{\sim}{z}_K)]$.

6.3 Problems with Bound on Output Estimation Error

In the monitoring problem with bound on the maximum allowable error in the estimate of the pollutant throughout the medium, it is necessary to make a measurement whenever for a time t_{K+N},

$$\max_{\underset{\sim}{z}} \sigma^2_{K+N}\left(\underset{\sim}{z}_K, \underset{\sim}{z}\right) \geq \sigma^2_{lim}, \tag{6.45}$$

where

$$\sigma^2_{K+N}\left(\underset{\sim}{z}_K, \underset{\sim}{z}\right) \equiv \underset{\sim}{c}(\underset{\sim}{z})^T \underset{\sim}{P}^K_{K+N}\left(\underset{\sim}{z}_K\right) \underset{\sim}{c}(\underset{\sim}{z}) \tag{6.46}$$

as in Section 5.4.1.

Suppose the first time (6.45) is satisfied is at sample time t_K. It is required to select the best set of measurement locations $\underset{\sim}{z}^*_K$ such that

$$\sigma^2_{K+N}\left(\underset{\sim}{z}^*_K, \underset{\sim}{z}^*\right) = \min_{\underset{\sim}{z}_K} \max_{\underset{\sim}{z}} \sigma^2_{K+N}\left(\underset{\sim}{z}_K, \underset{\sim}{z}\right) \tag{6.47}$$

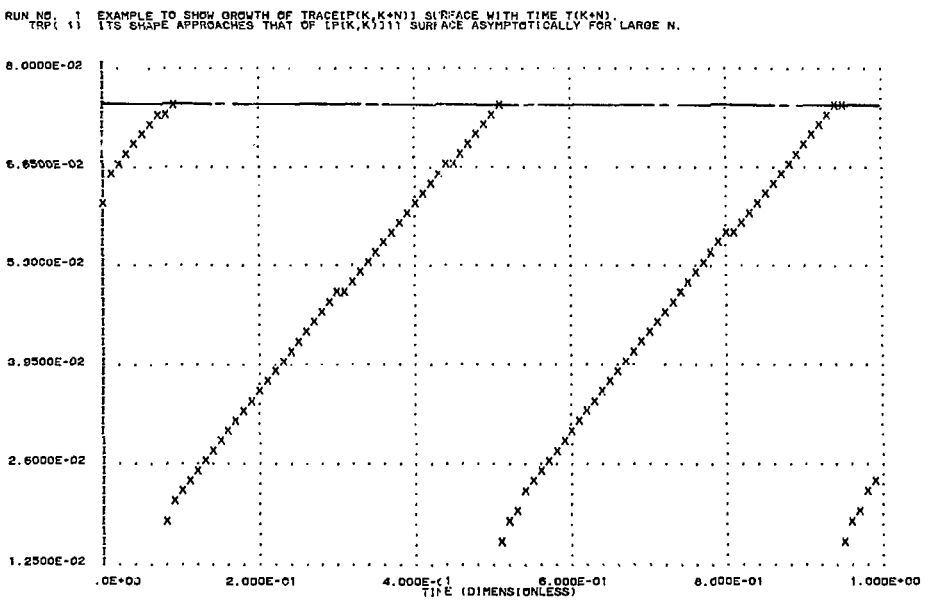


Figure 6.13. Time response of $\mathrm{Tr}\left[\underset{\sim}{P}^{K}_{K+N}\left(\underset{\sim}{z}^{*}_{K}\right)\right]$, showing three sample times at t_K = 0.09, 0.52, and 0.96.

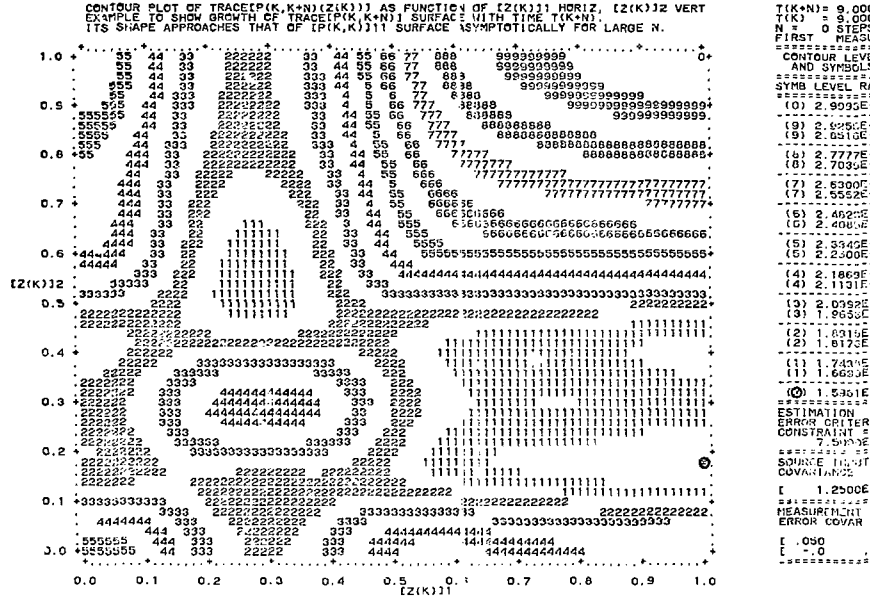


Figure 6.14. Contour plot of $\mathrm{Tr}\left[\underset{\sim}{P}_K(\underset{\sim}{z}_K)\right]$ at first measurement time, $t_K = 0.09$; compare with Figure 6.6 for case with different measurement error covariance matrix $\underset{\sim}{V}$.

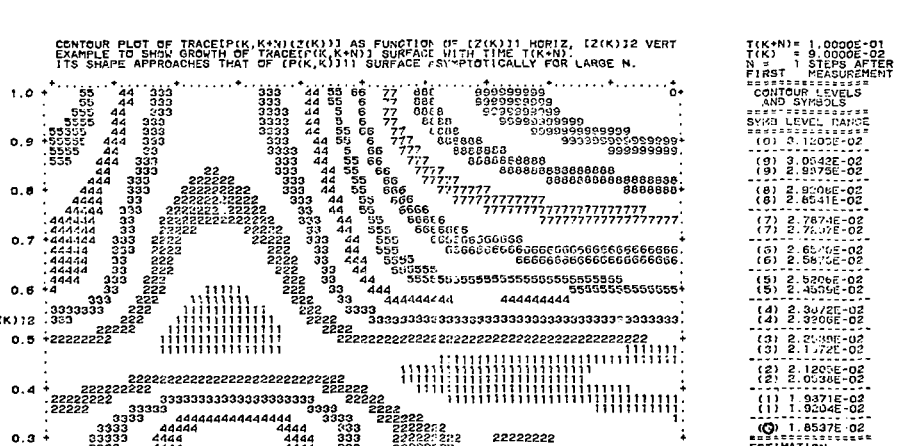


Figure 6.15A. Contour plot of $\mathrm{Tr}\left[P^{K}_{K+1}(z_K)\right]$ at time t_{K+1} = 0.10, one time step after first measurement.

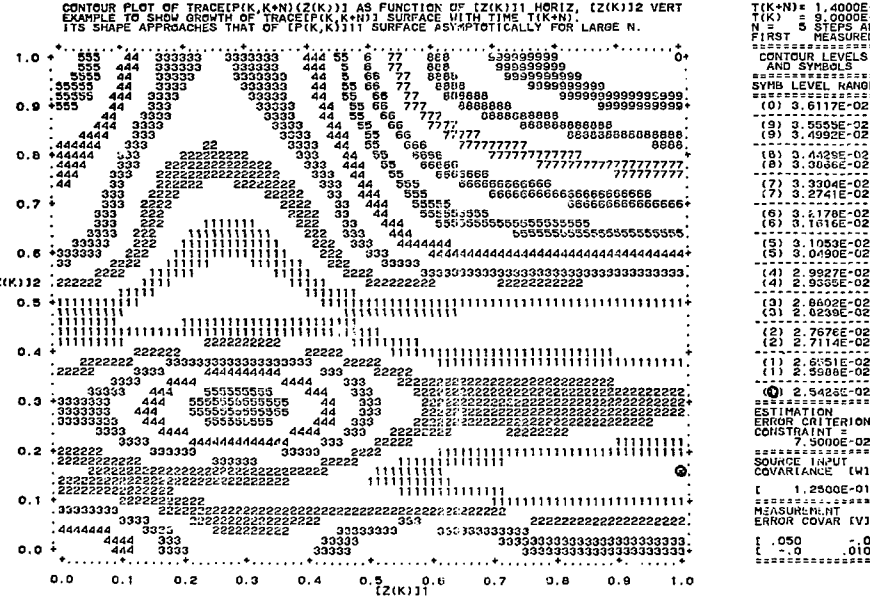
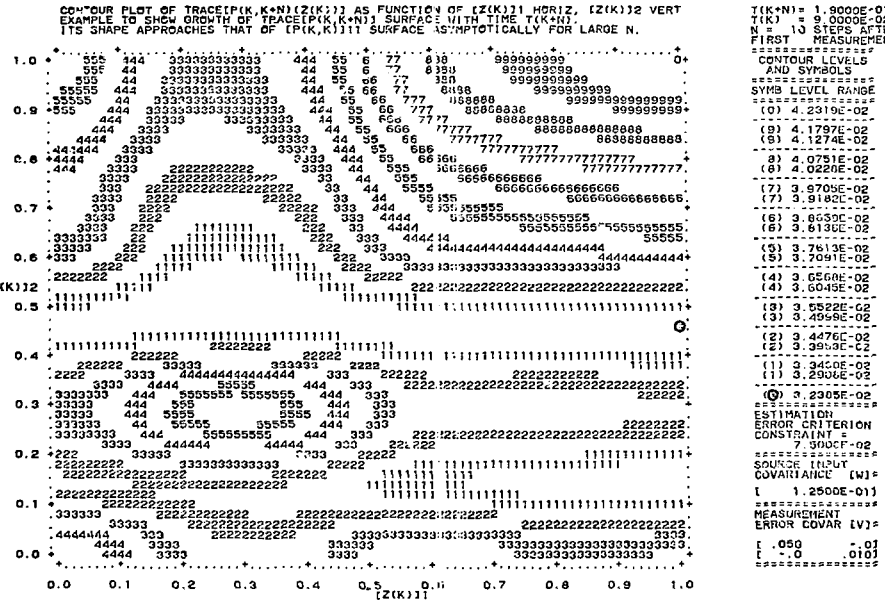


Figure 6.15B. Contour plot of $\mathrm{Tr}\left[P^{K}_{K+5}(\underline{z}_K)\right]$ at time t_{K+5} = 0.14, five time steps after first measurement.



T(K+N)= 1.9000E-01
T(K) = 9.0000E-02
N = 10 STEPS AFTER
FIRST MEASUREMENT

CONTOUR LEVELS AND SYMBOLS

SYMB	LEVEL RANGE
(0)	4.2319E-02
(9)	4.1797E-02
(8)	4.1274E-02
(8)	4.0751E-02
(8)	4.0228E-02
(7)	3.9705E-02
(7)	3.9182E-02
(6)	3.8659E-02
(6)	3.8136E-02
(5)	3.7613E-02
(5)	3.7091E-02
(4)	3.6568E-02
(4)	3.6045E-02
(3)	3.5522E-02
(3)	3.4999E-02
(2)	3.4476E-02
(2)	3.3953E-02
(1)	3.3430E-02
(1)	3.2906E-02
(0)	3.2385E-02

ESTIMATION ERROR CRITERION CONSTRAINT =
7.5000E-02

SOURCE INPUT COVARIANCE [W]=
[1.2500E-01]

MEASUREMENT ERROR COVAR [V]=
[.050 -.01
[-.0 .010]

Figure 6.15C. Contour plot of $\mathrm{Tr}\left[P^{K}_{K+10}(z_K)\right]$ at time t_{K+10} = 0.19, ten time steps after first measurement.

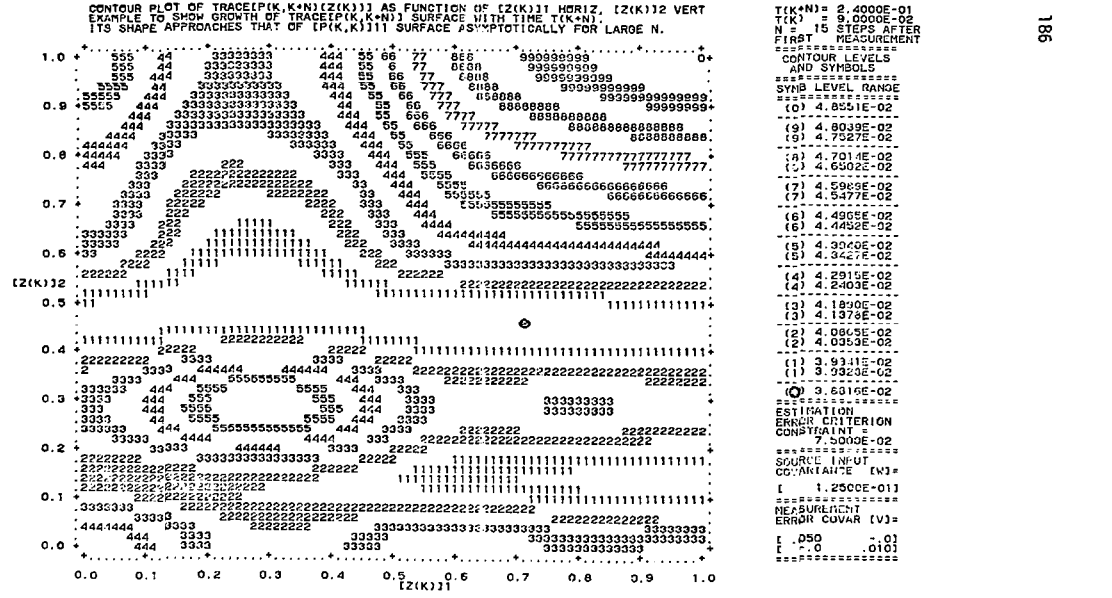


Figure 6.15D. Contour plot of $\mathrm{Tr}\left[\underset{\sim}{P}^{K}_{K+15}\left(\underset{\sim}{z}_{K}\right)\right]$ at time t_{K+15} = 0.24, fifteen time steps after first measurement.

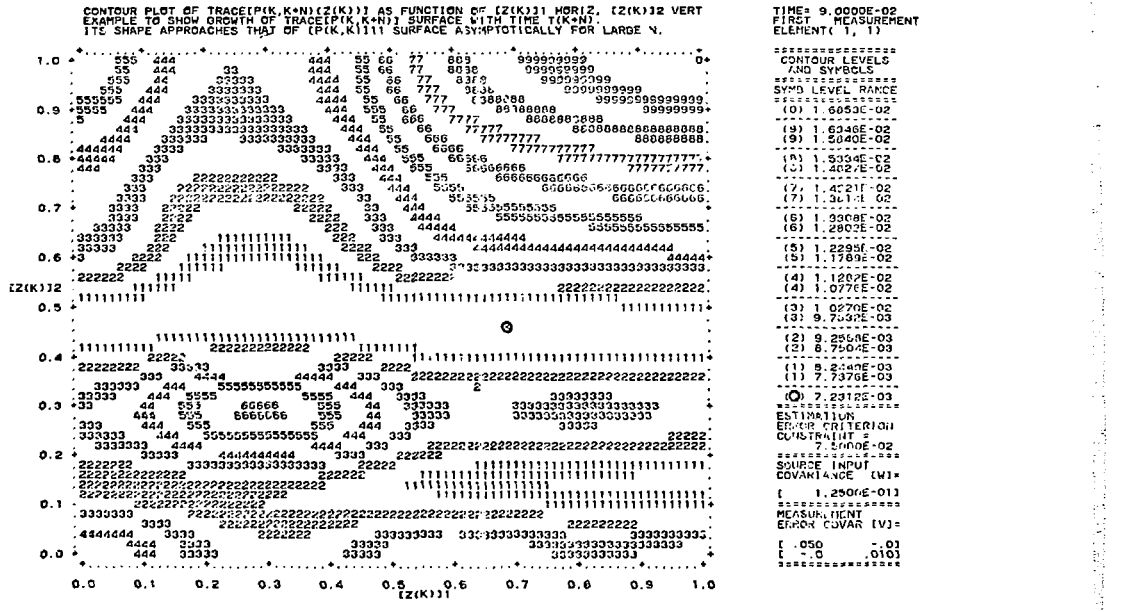


Figure 6.16. Contour plot of $\left[P_K^K(z_K)\right]_{11}$ at first measurement time, $t_K = 0.09$; compare with asymptotic response of $\mathrm{Tr}\left[P_{K+N}^K(z_K)\right]$ surface at $t_{K+15} = 0.24$ in Figure 6.15D.

at the next sample at time t_{K+N} when (6.45) is next satisfied. From Conclusion X, the minimax problem in (6.47) separates into finding $\underset{\sim}{z}_K^*$ such that

$$\left[\underset{\sim}{P}_K^K(\underset{\sim}{z}_K^*)\right]_{11} = \min_{\underset{\sim}{z}_K} \left[\underset{\sim}{P}_K^K(\underset{\sim}{z}_K)\right]_{11} \tag{6.48}$$

and independently finding that z^* which leads to

$$\max_{z} \underset{\sim}{c}(z)^T \sum_{n=1}^{N} \underset{\sim}{\Phi}^{n-1} \underset{\sim}{\Omega} \underset{\sim}{\Phi}^{n-1\,T} \underset{\sim}{c}(z) \tag{6.49}$$

for N large. Various properties of the solution of this problem are demonstrated by example in what follows.

6.3.1 Asymptotic Responses of Output Estimation Error — to demonstrate the asymptotic separation of the minimax problem in (6.47) into the independent problems of vector minimization in (6.48) and scalar maximization in (6.49), the problem of Section 6.1 was solved but as a monitoring problem of the second kind with

$$\underset{\sim}{P}_0^0 \equiv \begin{bmatrix} 0.05 & & & & \bigcirc \\ & 0.02 & & & \\ & & 0.00001 & & \\ & & & 0.00001 & \\ \bigcirc & & & & 0.00001 \end{bmatrix}, \tag{6.50}$$

and with the bound on maximum variance in the output estimate

$$\sigma^2_{\ell im} \equiv 0.1. \tag{6.51}$$

For this case, a plot of the evolution of $\sigma^2_{K+N}(\underset{\sim}{z}_K^*, z^*)$ in the minimax problem statement in (6.47) as a function of time t_{K+N} is shown in Figure 6.17.

The asymptotic separation of the minimax problem is demonstrated in Figures 6.18 and 6.19. The former is a plot of $\sigma^2_K(\underset{\sim}{z}_0, z)$ as a function of the position in the medium z for values of time t_K = 0, T, 2T, ..., 9T

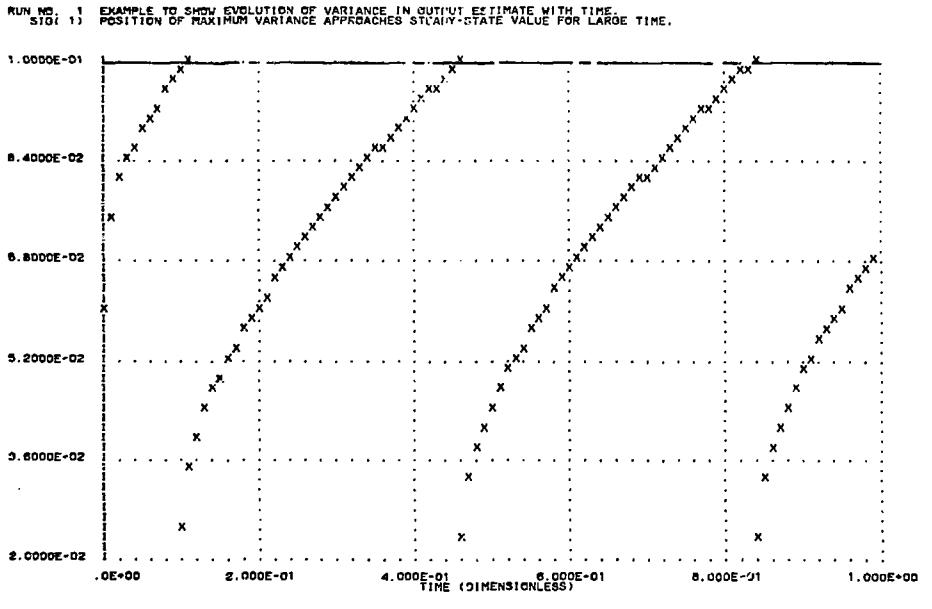


Figure 6.17. Time response of $\sigma^2_{K+N}\left(\xi^*_K, z^*\right)$, the performance criterion for the optimal monitoring problem with bound on error in the output estimate for $\sigma^2_{lim} \equiv 0.10$; samples occur at $t_K = 0.11$, 0.47, and 0.85.

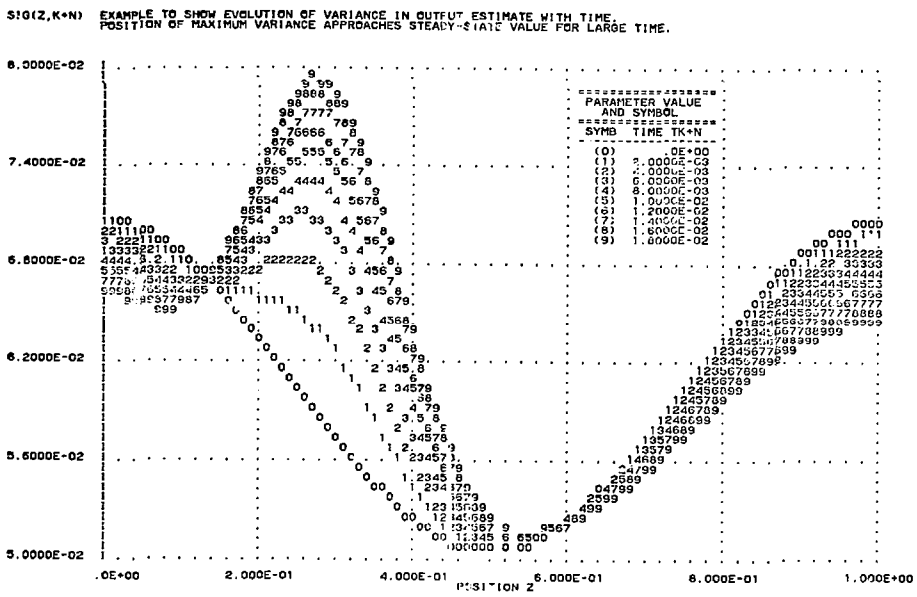


Figure 6.18. Plot of performance criterion $\sigma^2_{K+N}(z)$ as a function of position z in the medium for times $t_{K+N} = 0.0, 0.02, 0.04, \ldots 0.18$; note how position z^* of $\sigma^2_{K+N}(z^*) = \max_z \sigma^2_{K+N}(z)$ changes with time.

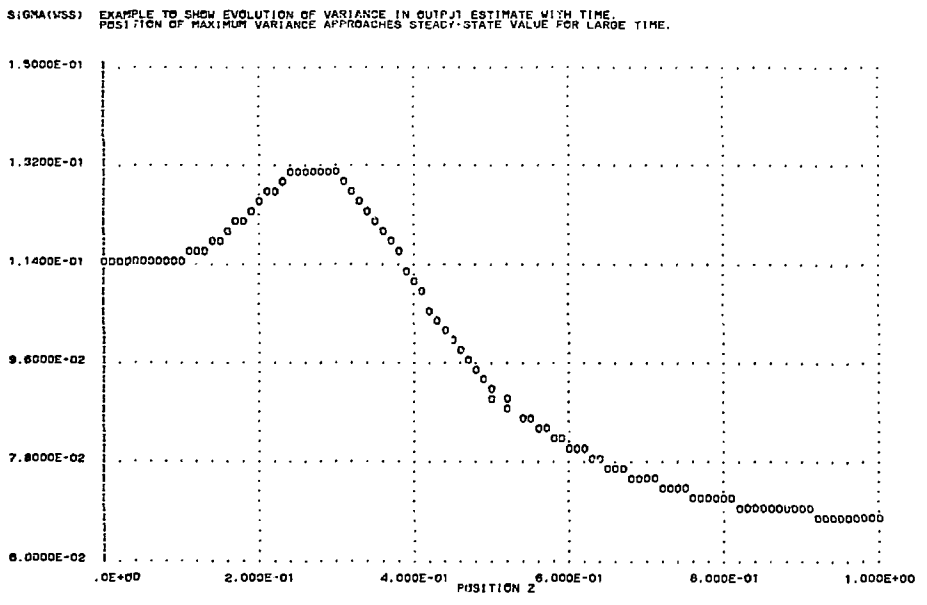


Figure 6.19. Plot of asymptotic shape of performance criterion $\sigma^2_{K+N}(z)$ as a function of position z in the medium as $N \to \infty$; compare position $z^* = 0.3$ for $\lim_{N\to\infty} \max_z \sigma^2_{K+N}(z)$ in this curve with asymptotic position of maximum in Figure 6.18.

where $T \equiv (t_{K+1} - t_K) = 0.002$. $\underset{\sim}{z}_0$ was taken as the initial guess at the best measurement locations, $\underset{\sim}{z}_0 \equiv [0.15, 0.15]^T$. The latter plot is a plot of

$$\underset{\sim}{c}(z)^T \underset{\sim SS}{\Omega} \underset{\sim}{c}(z), \tag{6.52}$$

the steady-state term in the asymptotic response of σ^2_{K+N} for N large. Thus, comparison of the asymptotic approach in time of the curves in Figure 6.18 to the steady-state curve in Figure 6.19 shows that

$$\underset{\sim}{c}(z)^T \sum_{n=1}^{N} \underset{\sim}{\Phi}^{n-1} \underset{\sim}{\Omega} \underset{\sim}{\Phi}^{n-1\,T} \underset{\sim}{c}(z) \rightarrow \underset{\sim}{c}(z)^T \underset{\sim SS}{\Omega} \underset{\sim}{c}(z). \tag{6.53}$$

As a special case, it shows that

$$\max_{z} \sigma^2_{K+N}(\underset{\sim}{z}_K, z) \longrightarrow \max_{z} \underset{\sim}{c}(z)^T \underset{\sim SS}{\Omega} \underset{\sim}{c}(z) \tag{6.54}$$

at the position of maximum variance z^*. Note here that as expected, the position of maximum variance is directly over the source position,

$$z^* = z_w. \tag{6.55}$$

6.3.2 The Effect of *a priori* Statistics — To demonstrate the effect of the uncertainty in the initial state estimate $\underset{\sim}{x}^0_0 \equiv \underset{\sim}{m}_0$ upon the optimal monitoring design problem, consider variations in the *a priori* statistics given in the initial state estimate error covariance matrix $\underset{\sim}{P}^0_0 \equiv \underset{\sim}{M}_0$. For this example, fix the time interval of interest at $0 \leq t \leq 2.0$ and set $\sigma^2_{lim} \equiv 0.2$.

Compare the first case for which

$$\underset{\sim}{P}^0_0 \equiv \underset{\sim}{M}_0 = \begin{bmatrix} 0.00001 & & \bigcirc \\ & \ddots & \\ \bigcirc & & 0.00001 \end{bmatrix}, \tag{6.56A}$$

with the case where

$$\underset{\sim}{P}_0^0 \equiv \underset{\sim}{M}_0 = \begin{bmatrix} 0.1 & & & \bigcirc \\ & 0.00001 & & \\ & & \ddots & \\ \bigcirc & & & 0.00001 \end{bmatrix}. \qquad (6.56B)$$

The first choice results in the evolution of $\sigma^2_{K+N}(\underset{\sim}{z}^*_K, z^*)$ shown in Figure 6.20, resulting in one measurement at $t_K = 1.26$. The corresponding contour plot of $[\underset{\sim}{P}^K_K(\underset{\sim}{z}_K)]_{11}$ as a function of $[\underset{\sim}{z}_K]_1$ and $[\underset{\sim}{z}_K]_2$ for that measurement is shown in Figure 6.21.

The plot of $\sigma^2_{K+N}(\underset{\sim}{z}^*_K, z^*)$ for the second choice of $\underset{\sim}{M}_0$ as in (6.56B) is shown in Figure 6.22, where owing to the higher initial value of σ^2_0, two sample times result at $t = 0.46$ and $t = 1.60$. The corresponding contour plots for those measurements are shown in Figure 6.23.

Study of Figures 6.21 and 6.23 show that the locations of optimal measurement positions are *not* effected by the *a priori* statistics given in $\underset{\sim}{M}_0$, provided that the time to the first sample is sufficiently long for the infrequent sampling approximations to apply.

For the first case, the time to the first sample is $t_K = 1.26$; for the second case, the first sample occurred at $t_K = 0.46$. Thus, the *only* effect that the choice of $\underset{\sim}{M}_0$ has upon the optimal monitoring design problem is the determination of the *time* of the first sample.

Thus, the results of Conclusion V are substantiated here within the context of a monitoring problem with bound on output estimation error.

To illustrate the transient effects at play in the general monitoring problem, effects that exist before the infrequent sampling requirements of (5.18) and (5.20) are met, consider the same problem as in the

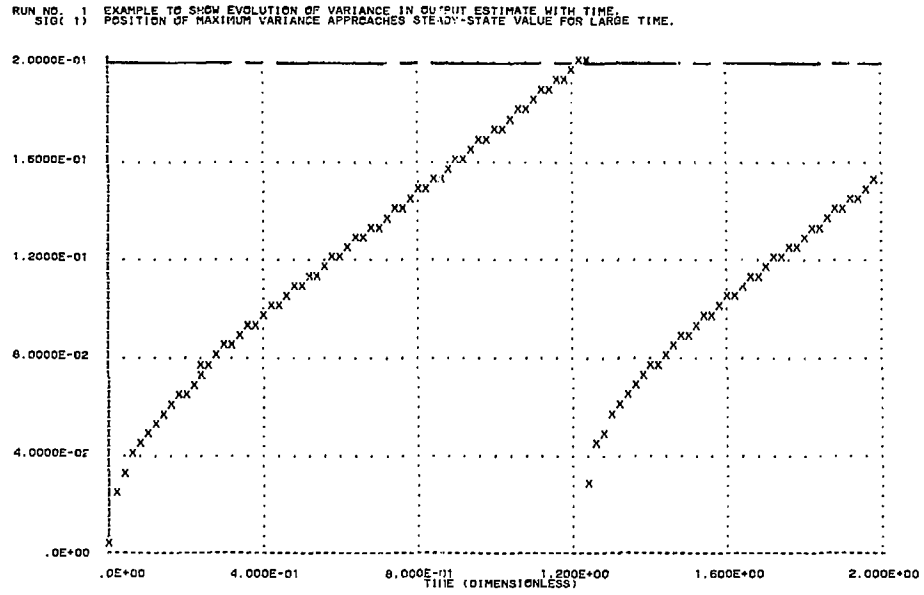


Figure 6.20. Time response of $\sigma^2_{K+N}\left(z^*_K, z^*\right)$ for $\sigma^2_{lim} \equiv 0.2$ with initial covariance matrix $P^0_{\sim 0} \equiv M_{\sim 0}$ given in (6.56A); one sample occurs at $t_K = 1.26$.

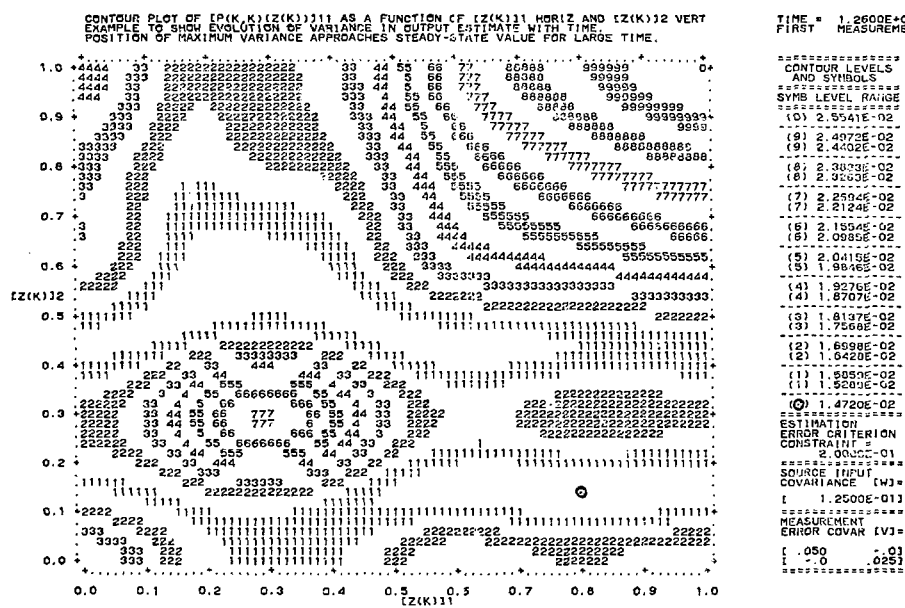


Figure 6.21. Contour plot of $\left[P_K^K(z_K)\right]_{11}$ with initial covariance matrix $P_0^0 \equiv M_0$ given in (6.56A) for the sample at $t_K \approx 1.26$.

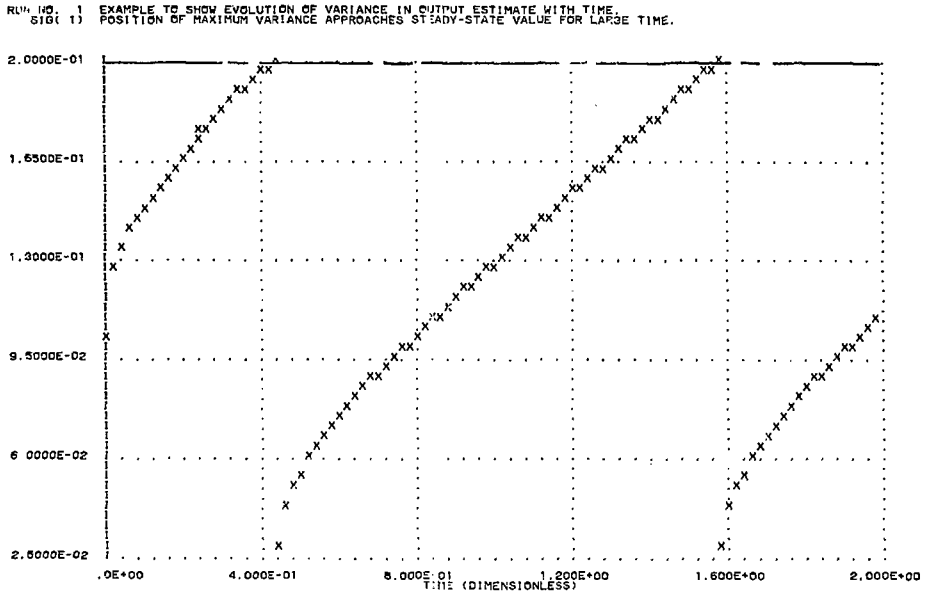


Figure 6.22. Time response of $\sigma^2_{K+N}(\underset{\sim}{z}^*_K, z^*)$ for $\sigma^2_{lim} \equiv 0.2$ with initial covariance matrix $\underset{\sim}{P}^0_0 \equiv \underset{\sim}{M}_0$ given in (6.56B); two samples occur at $t_K = 0.46$ and 1.60.

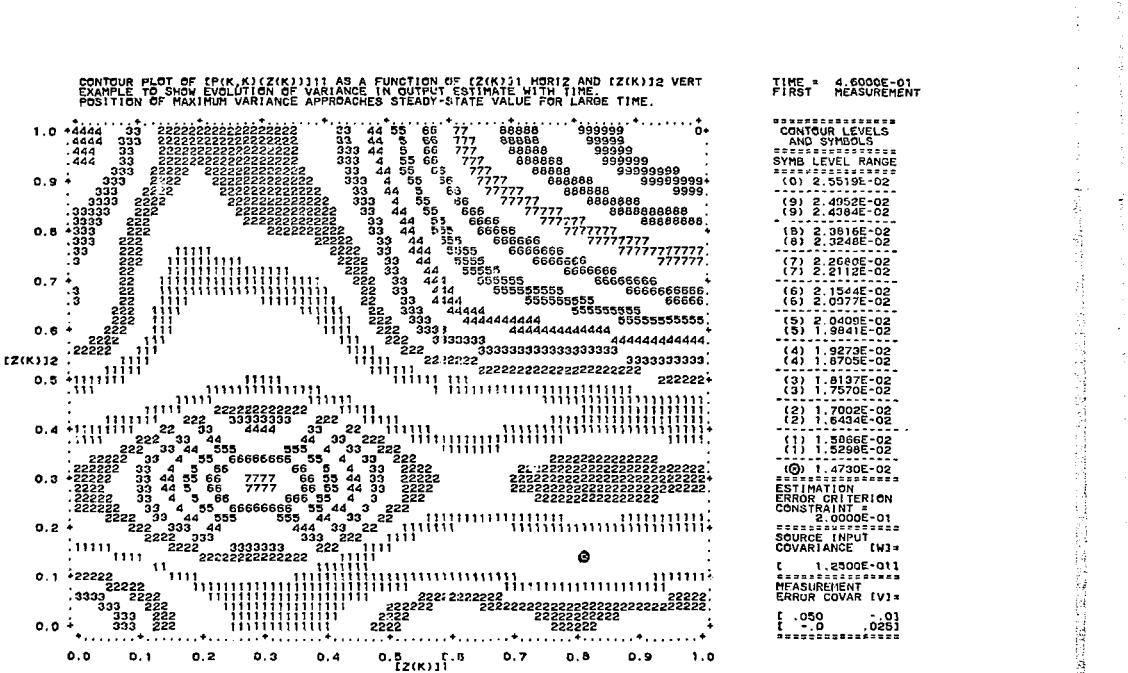


Figure 6.23A. Contour plot of $\left[P_K^K(z_K)\right]_{11}$ with initial covariance matrix $P_0^0 \equiv M_0$ given in (6.56B) and $\sigma_{lim}^2 \equiv 0.2$, for the first sample at $t_K = 0.46$.

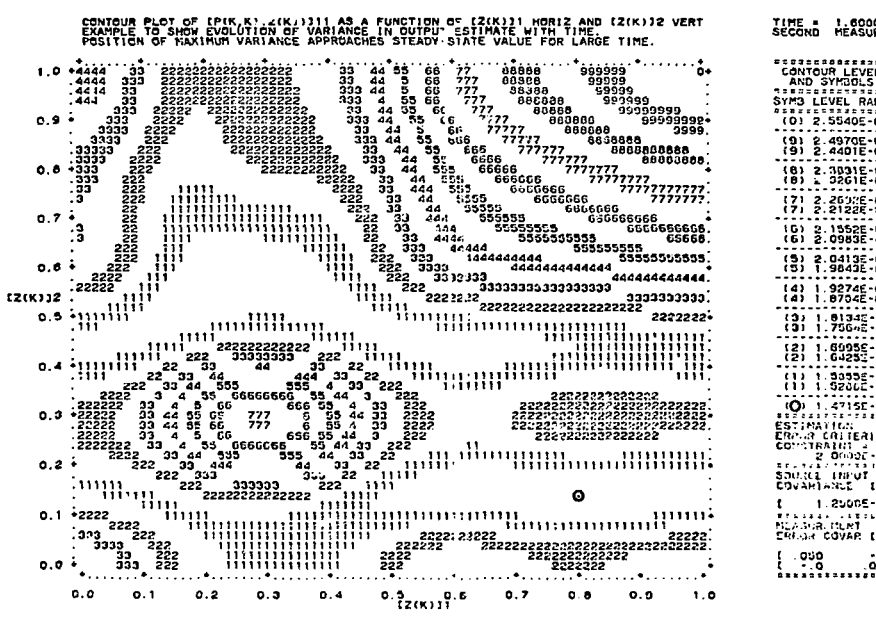


Figure 6.23B. Contour plot of $\left[P_{\underset{\sim}{K}}^{K}\left(\underset{\sim}{z}_K\right)\right]_{11}$ with initial covariance matrix $P_{\underset{\sim}{0}}^{0} \equiv \underset{\sim}{M}_0$ given in (6.56B) and $\sigma_{lim}^2 \equiv 0.2$, for the second sample at $t_K = 1.60$.

last case above with $\underset{\sim}{M}_0$ defined in (6.56B) but with $\sigma^2_{lim} \equiv 0.15$ instead. This results in the curve for $\sigma^2_{K+N}(\underset{\sim}{z}^*_K, z^*)$ shown in Figure 6.24 for the shorter time interval $0 \leq t \leq 1.0$. Two sample times result at $t_K = 0.11$ and $t_{K+N} = 0.86$. Corresponding plots for $[\underset{\sim}{P}^K_K(\underset{\sim}{z}_K)]_{11}$ and $[\underset{\sim}{P}^{K+N}_{K+N}(\underset{\sim}{z}_{K+N})]_{11}$ are given in Figure 6.25. Notice how in this case that the optimal measurement positions $\underset{\sim}{z}^*_K$ and $\underset{\sim}{z}^*_{K+N}$ at the two samples are *different*. The reason for this is that here, the estimation error limit σ^2_{lim} is so low that the infrequent sampling approximations do not apply at the first sample time. This is inferred by the response of $\sigma^2_{K+N}(\underset{\sim}{z}^*_K, z^*)$ in Figure 6.24 where it is seen that the steady-state slope $[\underset{\sim}{Q}]_{11} \equiv 0.00125$ for this problem has not been reached yet at the first sample whereas it has at the second; thus the steady-state simplifications do not apply at the first sample. For this reason, in practical applications, step (3) of the algorithmic procedure given in (5.72) is important where, at each sample, it is necessary to check whether or not steady-state conditions have been adequately approached for the infrequent sampling approximations to apply.

6.3.3 Problems with a Fixed Number of Samplers and Constant Error Bound — Consider a problem with $m = 2$ samplers to be used in every measurement with a time-invariant error bound $\sigma^2_{lim} \equiv 0.075$.

The initial covariance matrix

$$\underset{\sim}{P}^0_0 = \underset{\sim}{M}_0 \equiv \begin{bmatrix} 0.00001 & & \bigcirc \\ & \ddots & \\ \bigcirc & & 0.00001 \end{bmatrix}. \tag{6.57}$$

Conclusion V and XI are substantiated in the context of this problem with bound on output error.

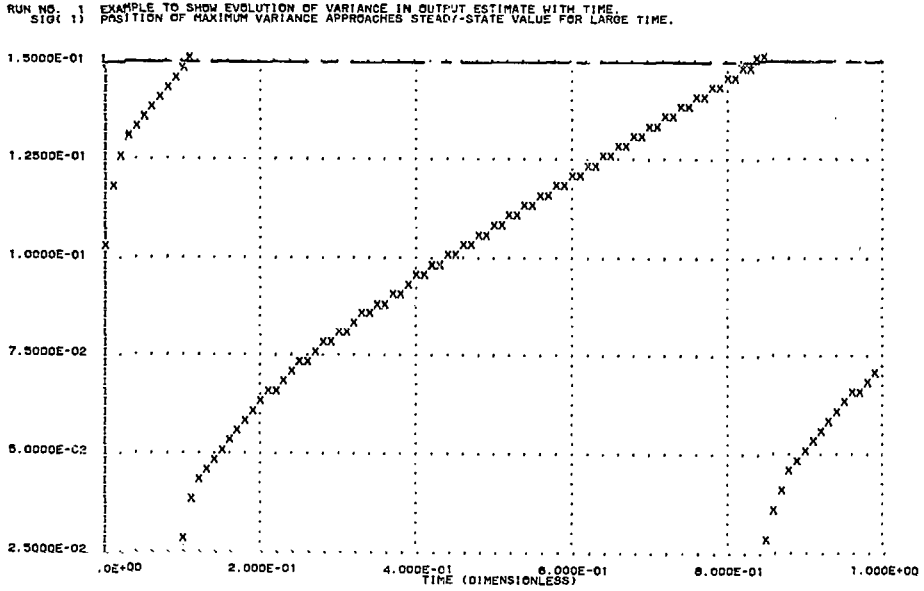


Figure 6.24. Time response of $\sigma^2_{K+N}\left(z^*_K, z^*\right)$ for $\sigma^2_{lim} \equiv 0.15$ with initial covariance matrix $\underset{\sim}{P}^0_0 \equiv \underset{\sim}{M}_0$ given in (6.56B). Two samples occur at $t_K = 0.11$ and 0.86; compare with Figure 6.22 for case with $\sigma^2_{lim} \equiv 0.2$.

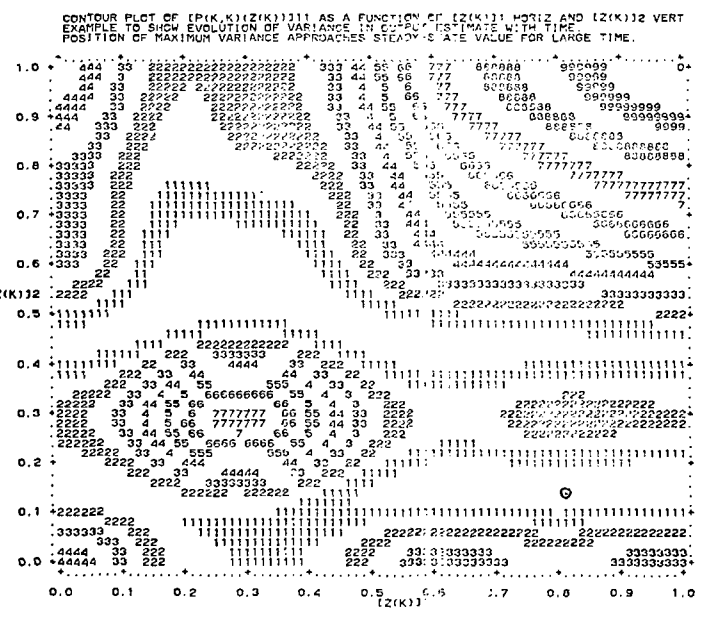


Figure 6.25A. Contour plot of $\left[\underset{\sim}{P}_K^K(\underset{\sim}{z}_K)\right]_{11}$ with initial covariance matrix $\underset{\sim}{P}_0^0 \equiv \underset{\sim}{M}_0$ given in (6.56B) and $\sigma^2_{lim} \equiv 0.15$ for the first sample at $t_K = 0.11$. Compare with Figure 6.23A for case with $\sigma^2_{lim} \equiv 0.2$.

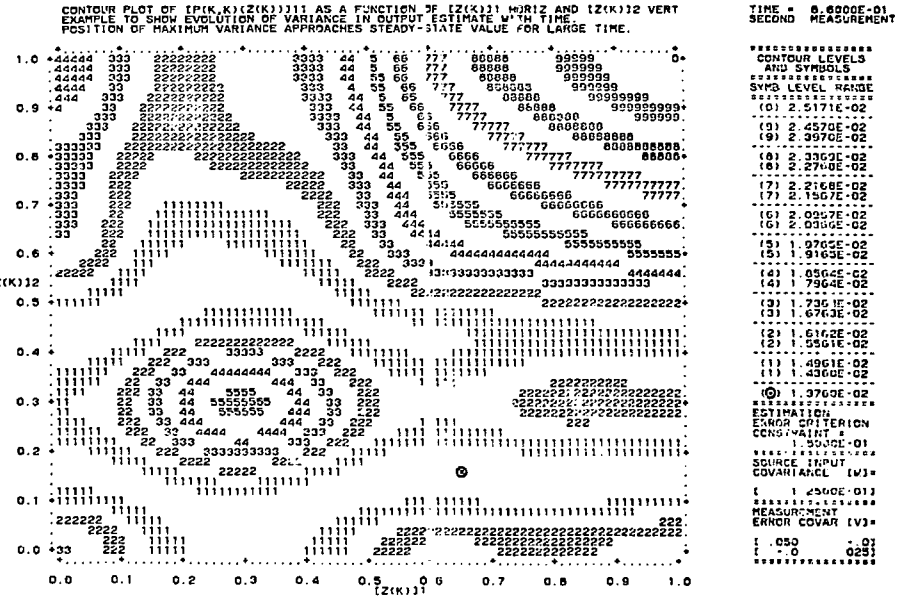


Figure 6.25B. Contour plot of $\left[P_{\underset{\sim}{K}}^{K}(\underset{\sim}{z}_K)\right]_{11}$ with initial covariance matrix $P_{\underset{\sim}{0}}^{0} \equiv M_{\underset{\sim}{0}}$ given in (6.56B) and $\sigma_{lim}^2 = 0.15$ for the second sample at $t_K = 0.86$. Compare with Figure 6.23B for case with $\sigma_{lim}^2 \equiv 0.2$.

Suppose the problem starts at time t_0. As discussed in Section 6.3, and according to Conclusion XI, the position z^* of maximum variance in the estimate of the pollutant concentration at all measurement times is independent of time and is thus calculated at the beginning of the problem. With this value z^*, relationships among the various optimal measurement position vectors $\underset{\sim}{z}^*$ at the measurement times are to be considered.

Assume that the time the first measurement is required is at time t_K. $\underset{\sim}{z}_K^*$ is found to maximize t_{K+N}, the time the next measurement is required. Then, at t_{K+N}, $\underset{\sim}{z}_{K+N}^*$ is found to maximize the next time interval to a measurement, etc. A typical plot of $\sigma^2(\underset{\sim}{z}^*,z^*)$ over values of t_K is shown in Figure 6.26. For each measurement time t_{K+N}, $\underset{\sim}{z}_{K+N}^*$ is to be found to minimize $[\underset{\sim}{P}_{K+N}^{K+N}(\underset{\sim}{z}_{K+N})]_{11}$ so that to corroborate the optimizations over $\underset{\sim}{z}_{K+N}$, contour plots are made at every measurement time for $[\underset{\sim}{P}_{K+N}^{K+N}(\underset{\sim}{z}_{K+N})]_{11}$ as a function of $[\underset{\sim}{z}_{K+N}]_1$ horizontally and $[\underset{\sim}{z}_{K+N}]_2$ vertically. Plots for the four resulting measurement times in this problem at t = 0.27, 0.48, 0.69, and 0.90 are shown in Figure 6.27. Notice that the contours at all samples are the same, leading to the *same* optimal design for $\underset{\sim}{z}_{K+N}^*$ at all measurement times t_{K+N}; thus, Conclusion VI is demonstrated.

Comparing the first two measurement time intervals in Figure 6.26, that is, $(t_K - t_0) = 0.27$ compared with $(t_{K+N} - t_K) = 0.21$ shows that, for N large, the *only* effect that the choice of M_0 has upon the optimal measurement design at the first sample at time t_K is in determining the *time* of the required measurement, t_K; it has no effect upon the optimal *locations* $\underset{\sim}{z}_K^*$ which demonstrates again Conclusion V.

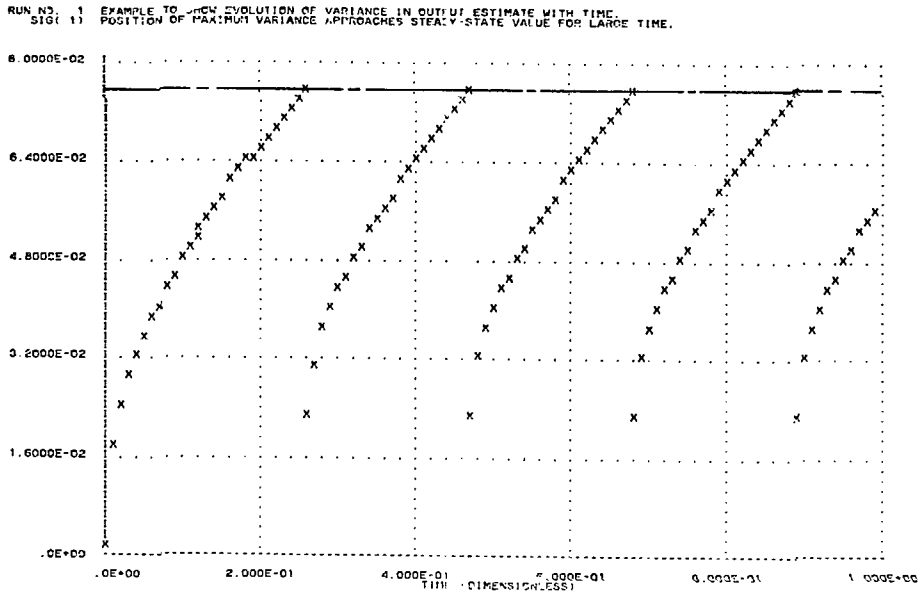


Figure 6.26. Time response of $\sigma^2_{K+N}(z^*_K, z^*)$ for $\sigma^2_{\text{max}} = 0.075$; four samples occur at t_K = 0.27, 0.48, 0.69, and 0.90.

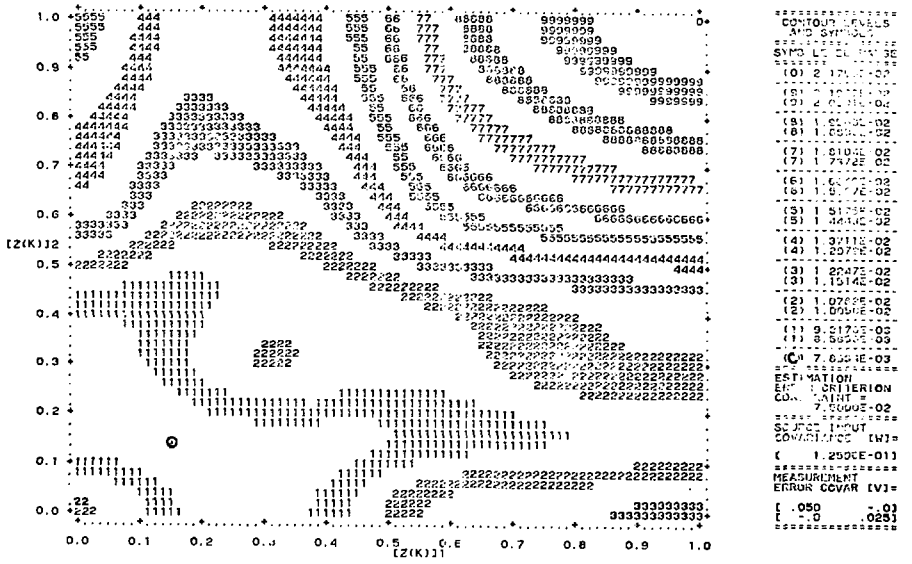


Figure 6.27A. Contour plot of $\left[P_{K}^{K}(\underset{\sim}{z}_{K})\right]_{11}$ for the first sample at $t_K = 0.27$.

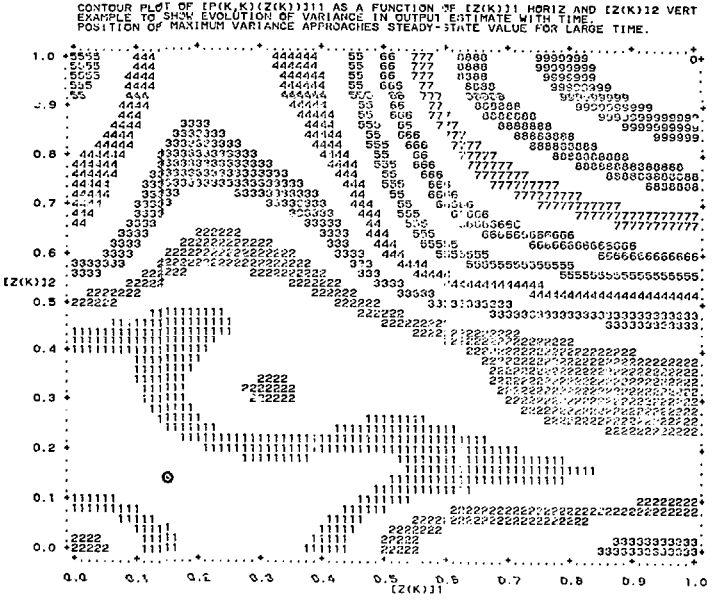


Figure 6.27B. Contour plot of $\left[P_K^K(z_K)\right]_{11}$ for the second sample at $t_K = 0.48$.

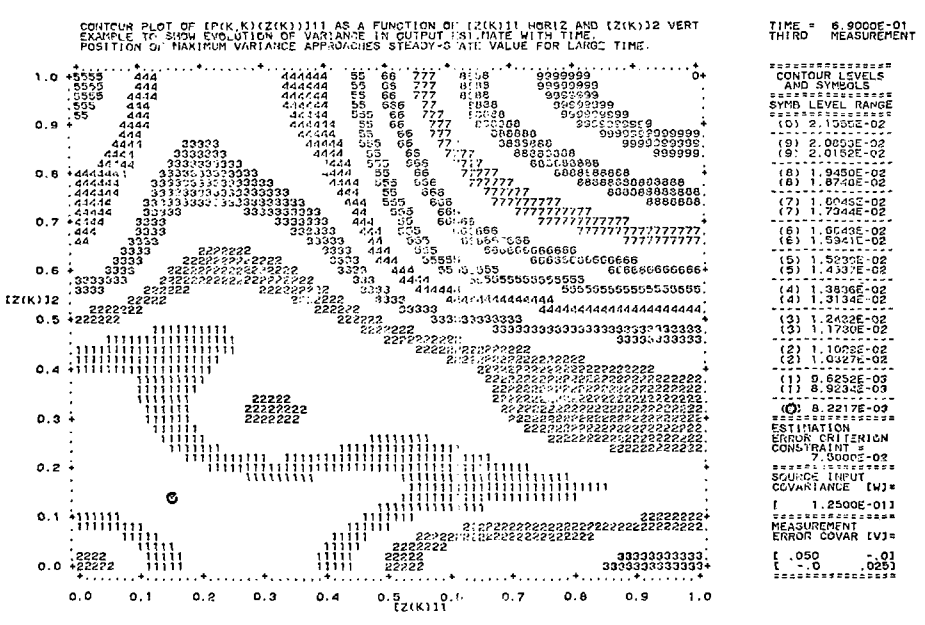


Figure 6.27C. Contour plot of $\left[P_K^K(z_K)\right]_{11}$ for the third sample at $t_K = 0.69$.

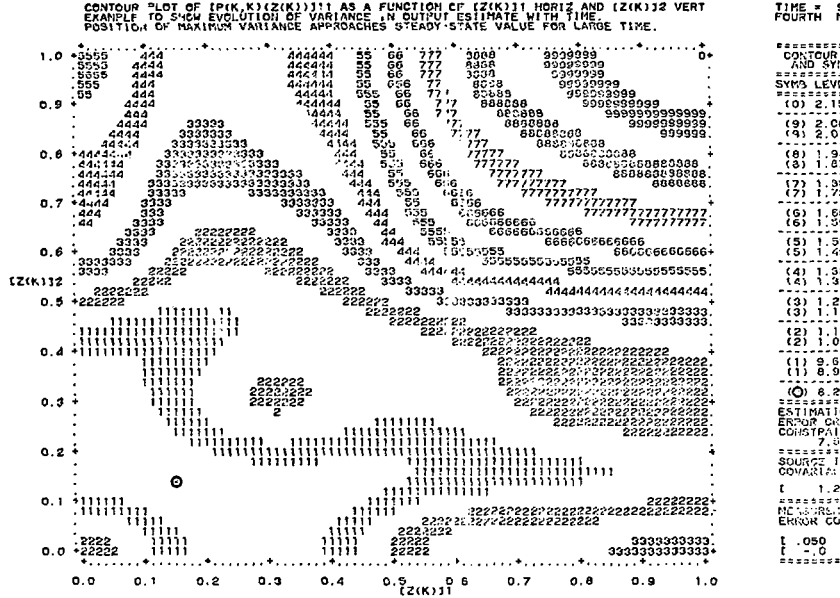


Figure 6.27D. Contour plot of $\left[P_K^K(z_K)\right]_{11}$ for the fourth sample at $t_K = 0.90$.

6.3.4 The Effect of Level of Estimation Error Bound upon the Optimal Monitoring Problem — In the examples of the previous two sections, a comparison is now made of the effect of the level of the estimation error limit σ^2_{lim} upon the outcomes of the optimal monitoring problems of design and management. In both cases, start with M_0 given in (6.56A) or (6.57). In the first example in Section 6.3.2, $\sigma^2_{lim} = 0.2$ whereas in that of Section 6.3.3, $\sigma^2_{lim} = 0.075$.

In the first case, $\sigma^2_{K+N}(\underline{z}^*_K, z^*)$ is shown in Figure 6.20, in the second, in Figure 6.26. Notice immediately that there is a *direct* effect upon the monitoring problem; a lower estimation error limit leads to higher sampling frequency as would be expected.

However, a more interesting point comes in the effect of the value of σ^2_{lim} upon the optimal *design* problem, the optimal placement of monitors. Comparison of the contour plots of $[\underline{P}^K_K(\underline{z}_K)]_{11}$ for sample times t_K in Figure 6.21 for $\sigma^2_{lim} \equiv 0.2$ with those in Figure 6.27 for $\sigma^2_{lim} \equiv 0.075$ shows that the optimal design problems are vastly different leading to entirely different positions $\underline{z}^*_K$ for the global minima in the two problems.

Notice also that the shape of the contour in Figure 6.21 is different from those in 6.27, the predominant difference being the smaller height of the rise around the source location $z_w \equiv 0.3$. This can be explained as follows. In the case of the first samples, for the problem with $\sigma^2_{lim} \equiv 0.075$, $t_K = 0.27$ whereas for $\sigma^2_{lim} \equiv 0.20$, $t_K = 1.26$. Thus, the stochastic source has longer to act upon the system with the higher error bound. The effect of this can be seen by considering the form of the predicted covariance matrix $\underline{P}^0_K$ in (6.24) and (6.28). For the asymptotic case of infrequent sampling, from Section 5.3.2,

$$\begin{bmatrix} \\ \underset{\sim}{P}_K^0 \\ \\ \end{bmatrix} = \begin{bmatrix} [\underset{\sim}{M}_0]_{11} & \\ & \bigcirc \end{bmatrix} + \begin{bmatrix} K[\underset{\sim}{\Omega}]_{11} & \\ & \bigcirc \end{bmatrix} + \begin{bmatrix} 0 & \\ & \underset{SS}{\Omega} \end{bmatrix}, \quad (6.28)$$

or

$$\begin{bmatrix} \\ \underset{\sim}{P}_K^0 \\ \\ \end{bmatrix} = \begin{bmatrix} \left([\underset{\sim}{M}_0]_{11} + K[\underset{\sim}{\Omega}]_{11}\right) & \\ & \underset{SS}{\Omega} \end{bmatrix}. \quad (6.58)$$

Thus, as K grows, the first element of $\underset{\sim}{P}_K^0$ get larger relative to the other steady-state terms in $\underset{\sim}{P}_K^0$ as seen on the right-hand side of (6.58). This results in different values for the inverse $[\underset{\sim}{C}(z_K)\underset{\sim}{P}_K^0\underset{\sim}{C}(z_K)^T + \underset{\sim}{V}]^{-1}$ in the equation for the corrected covariance matrix in (6.26). Thus, with $T \equiv (t_{K+1} - t_K) = 0.01$, $\sigma^2_{lim} \equiv 0.2$ leads to K = 126 for the problem in Section 6.3.3 whereas that in 6.32 with $\sigma^2_{lim} \equiv 0.075$ leads to K = 27; this results in the different contours in Figures 6.21 and 6.27. Thus, the optimal design of the measurement locations is seen to be a function of the level of the error bound, which substantiates Conclusion IV.

6.3.5 Examples of Various Levels of Bound upon Output Error — The same problem as in the last examples was solved but with a range of error bound levels as follows: $\sigma^2_{lim} \equiv 0.05$, 0.075, 0.1, 0.125, 0.15, 0.2, and 0.5. Resultant contours of $[\underset{\sim}{P}_K^K(z_K)]_{11}$ at the first sample time t_K for each case are shown in Figure 6.28.

As the time interval grows before a sample is made, the uncertainty in the estimate of the state in the area near the source, $z_w \equiv 0.3$, becomes large relative to that elsewhere in the medium. These plots further

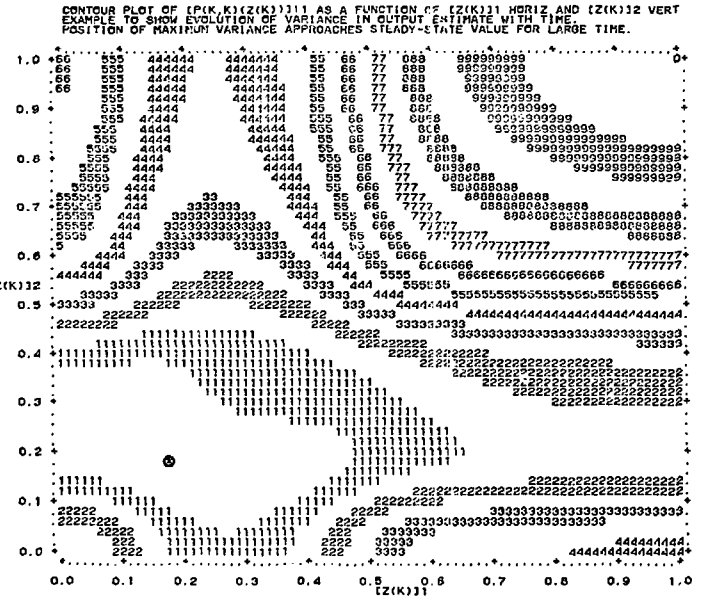


Figure 6.28A. Contour plot of $\left[P_K^K(z_K)\right]_{11}$ at first sample time $t_K = 0.11$ for $\sigma^2_{lim} \equiv 0.05$.

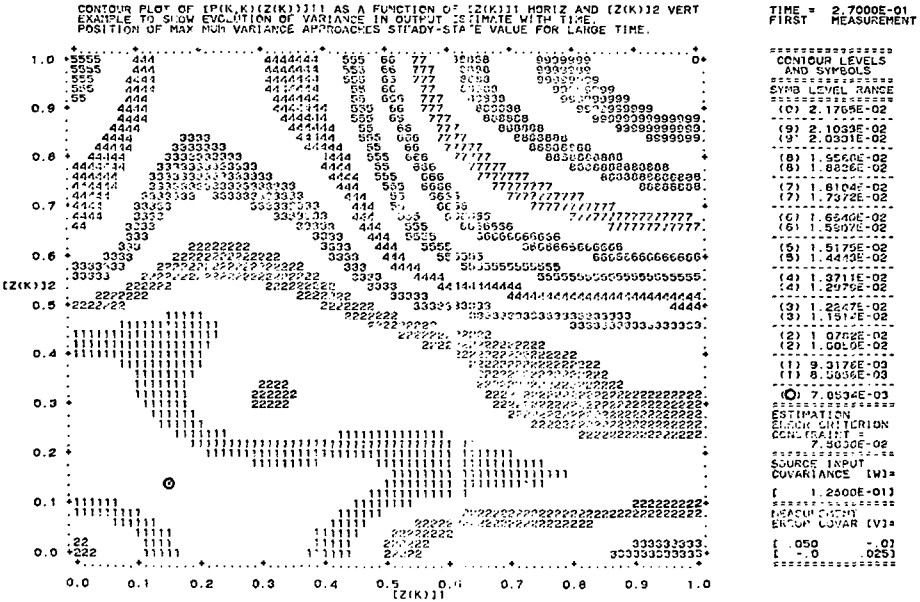


Figure 6.28B. Contour plot of $\left[P_{\underset{\sim}{K}}^{K}\left(\underset{\sim}{z}_K\right)\right]_{11}$ at first sample time $t_K = 0.27$ for $\sigma_{lim}^2 \equiv 0.075$.

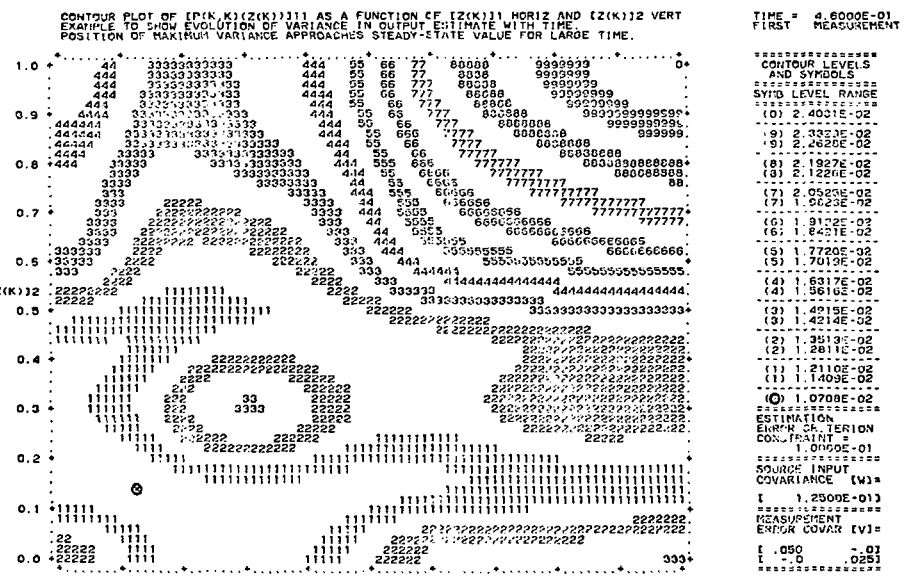


Figure 6.28C. Contour plot of $\left[P_K^K(z_K)\right]_{11}$ at first sample time $t_K = 0.46$ for $\sigma^2_{lim} = 0.10$.

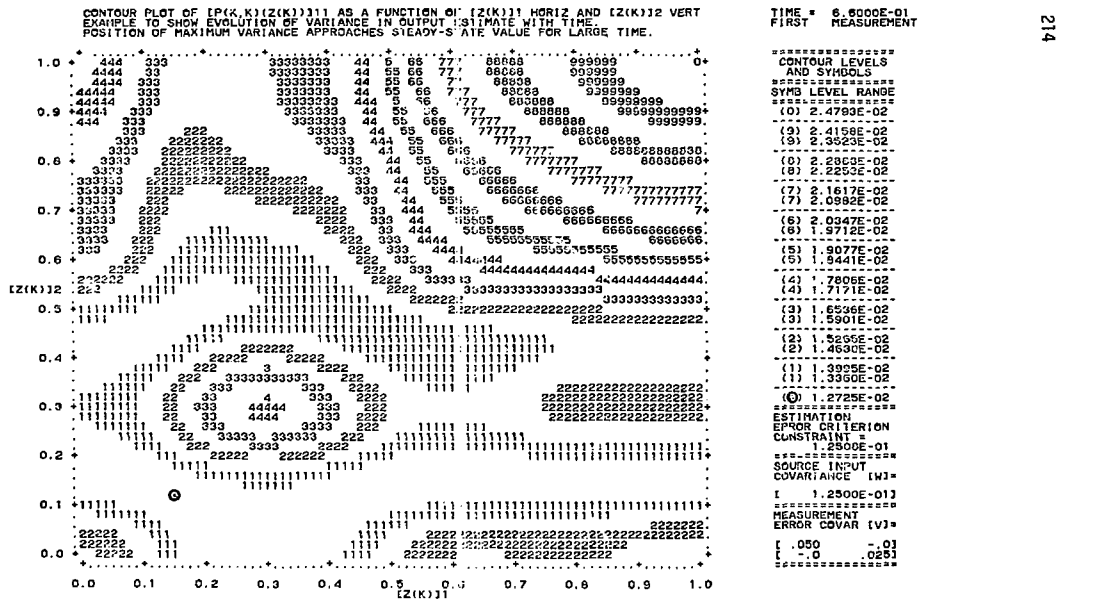


Figure 6.28D. Contour plot of $\left[\underset{\sim}{P}^{K}_{K}(\underset{\sim}{z}_{K})\right]_{11}$ at first sample time $t_K = 0.66$ for $\sigma^2_{lim} \equiv 0.125$.

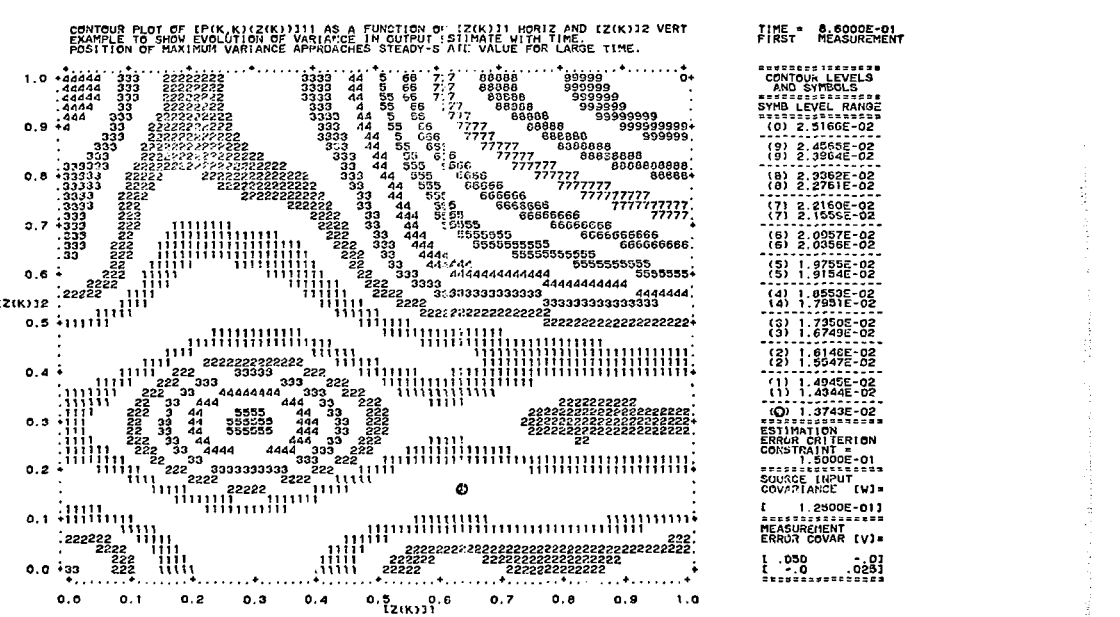


Figure 6.28E. Contour plot of $\left[\underline{P}_K^K\left(\underline{z}_K\right)\right]_{11}$ at first sample time $t_K = 0.86$ for $\sigma^2_{lim} = 0.15$.

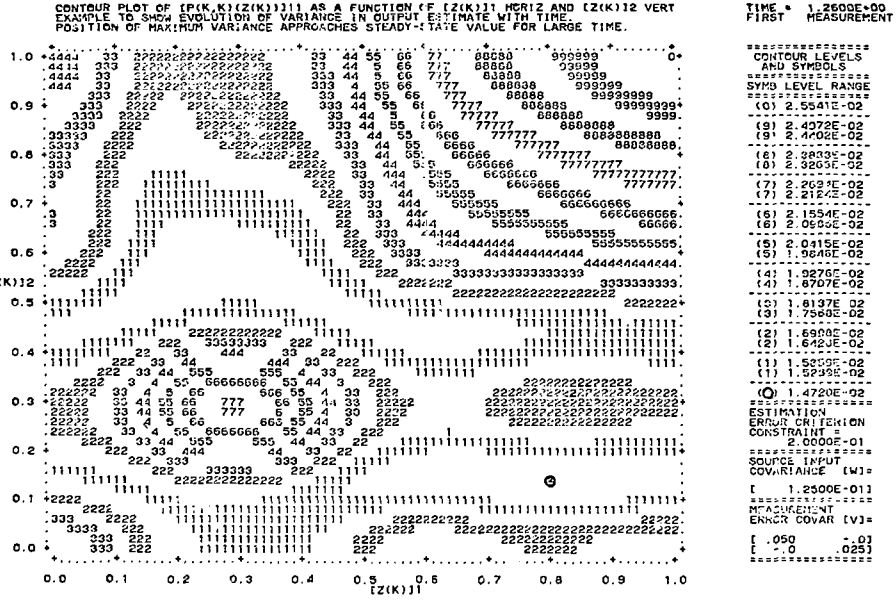


Figure 6.28F. Contour plot of $\left[P_K^K(z_K)\right]_{11}$ at first sample time $t_K = 1.26$ for $\sigma^2_{lim} \equiv 0.20$.

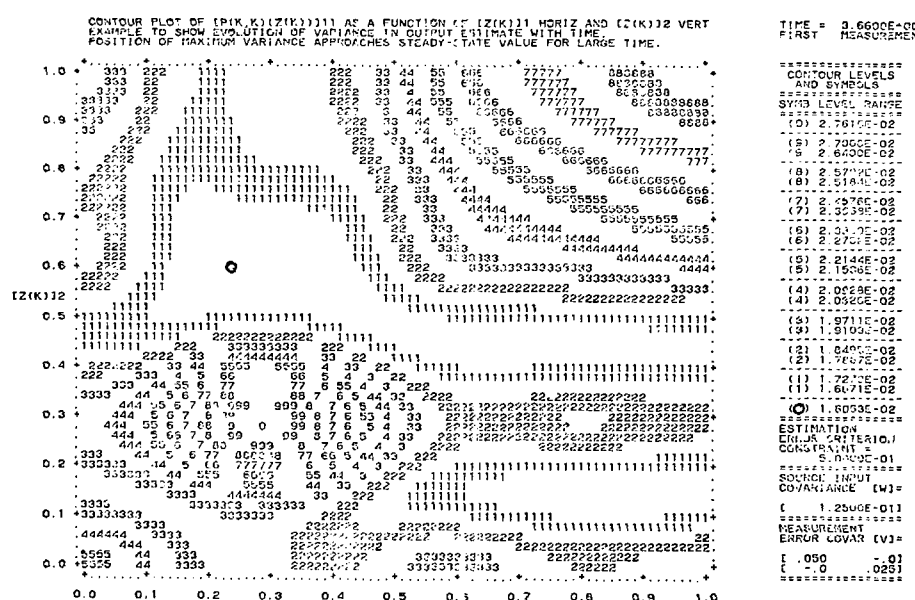


Figure 6.28G. Contour plot of $\left[P_K^K(z_K)\right]_{11}$ at first sample time $t_K = 3.66$ for $\sigma^2_{lim} = 0.50$.

substantiate the existence of a functional relationship between the optimal measurements $\underset{\sim}{z}_K^*$ and the level of the output error bound σ_{lim}^2.

6.3.6 The Effect of Time-Varying Error Bound upon the Optimal Measurement Design — Consider here an example where the output estimatior error limit σ_{lim}^2 is allowed to vary in time. For this problem, let

$$\sigma_{lim}^2 = 0.1 \tag{6.59}$$

at the first sample time and then

$$\sigma_{lim}^2 = \sigma_{lim}^2 + 0.025 \tag{6.60}$$

for each sample thereafter.

The resultant plot of $\sigma_{K+N}^2(\underset{\sim}{z}_K^*, \underset{\sim}{z}^*)$ over time for the interval $0 \leq t \leq 2$ is shown in Figure 6.29, where the initial covariance $\underset{\sim}{P}_0^0 \equiv \underset{\sim}{M}_0$ is as before in (6.57).

Notice how the curve asymptotically approaches the slope $[\underset{\sim}{\Omega}]_{11} = 0.0025$ just before each sample, in accordance with the infrequent sampling approximations.

At each sample, contour plots of $[\underset{\sim}{P}_K^K(\underset{\sim}{z}_K)]_{11}$ are generated and presented in Figure 6.30 for sample times $t_K = 0.46, 1.04, 1.80$. As can be seen from these plots, the contours change with the error level as shown in the previous sections; in fact, they directly compare with those of the previous section. Thus, the converse of Conclusion VI may be stated as

> Conclusion VIB. The optimal measurements found at one measurement time may not in general be optimal for other measurement times if the bound on estimation error varies with time. (C.VIB)

Further verifications of the effects of the *a priori* statistics and level of estimation error bound upon the optimal design problem can be

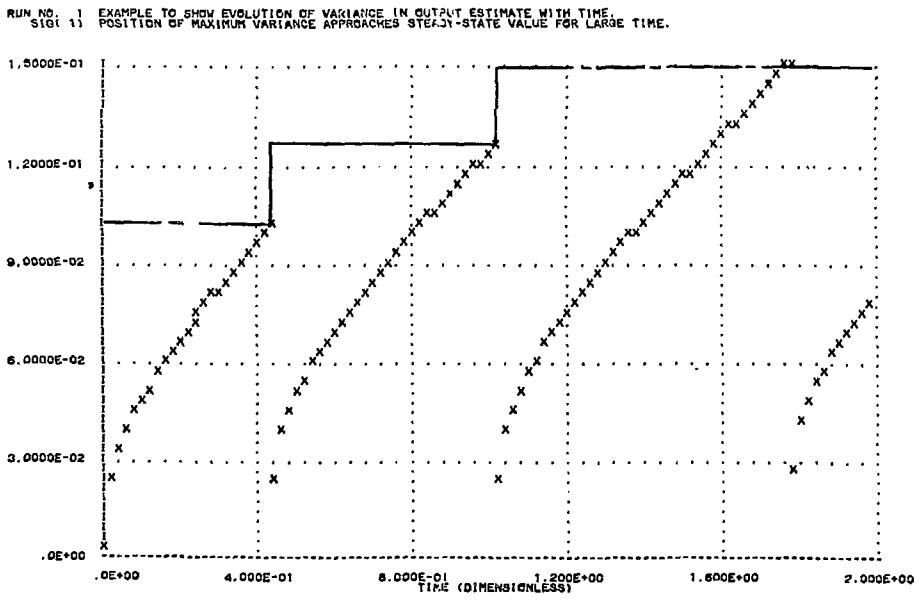


Figure 6.29. Time response of $\sigma^2_{K+N}\left(\underset{\sim}{z}^*_K, z^*\right)$ for time varying estimation error limit $\sigma^2_{lim}(t)$ = 0.10, 0.125, and 0.150 at sample times t_K = 0.46, 1.04, and 1.80, respectively.

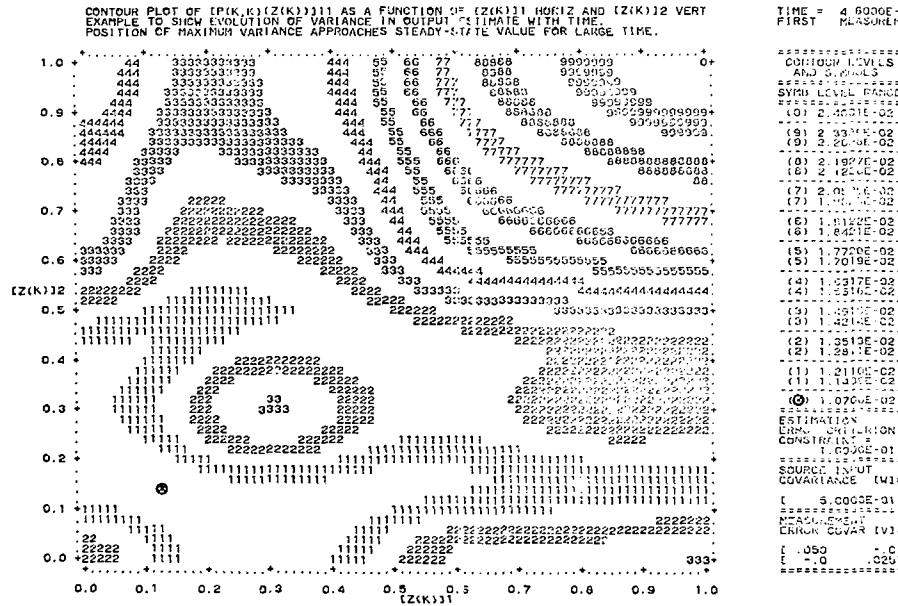


Figure 6.30A. Contour plot of $\left[P_k^K(z_K)\right]_{11}$ at first sample time $t_K = 0.46$ for $\sigma^2_{\tilde{z}_{1m}} = 0.10$; compare with Figure 6.28C.

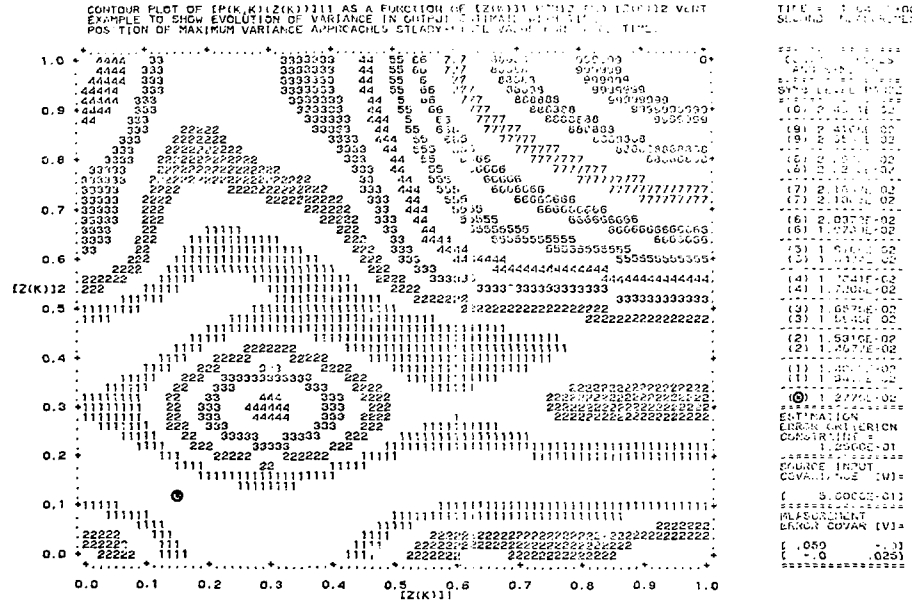


Figure 6.30B. Contour plot of $\left[P_K^K(z_K)\right]_{11}$ at second sample time $t_K = 1.04$ for $\sigma^2_{Z\,in} = 0.125$; compare with Figure 6.28D.

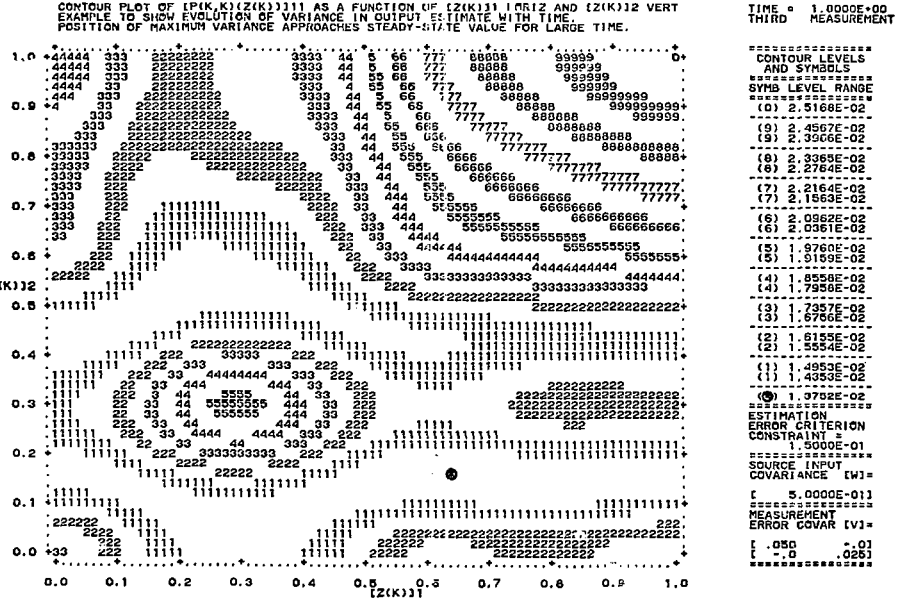


Figure 6.30C. Contour plot of $\left[P_K^K(z_K)\right]_{11}$ at third sample time $t_K = 1.80$ for $\sigma^2_{lim} = 0.150$; compare with Figure 6.28E.

obtained by comparison of the contours in Figure 6.30 with those for the cases with $\sigma^2_{\ell im} = 0.1$, 0.125, and 0.5 in Figure 6.28 in the previous section.

6.3.7 The Effect of Time-Varying Disturbance and Measurement Statistics upon the Optimal Monitoring Design and Management Problems — Consider a problem with

$$\sigma^2_{\ell im} \equiv 0.1, \tag{6.61A}$$

$$\underset{\sim}{W} \equiv 0.125, \tag{6.61B}$$

$$\underset{\sim}{V} \equiv \begin{bmatrix} 0.05 & 0 \\ 0 & 0.025 \end{bmatrix} \tag{6.61C}$$

and with $\underset{\sim}{P}^0_0 \equiv \underset{\sim}{M}_0$ given in (6.57). Consider two cases. First, fix the measurement statistics $\underset{\sim}{V}$ to the values given above in (6.61C) but let the disturbance statistics vary. For this case, for the time interval $0 \le t \le 2$, sample times occur at $t_K = 0.46$ and 1.22. The time-varying disturbance statistics between samples, starting with $\underset{\sim}{W}$ in (6.61B) is then given by

$$\underset{\sim}{W}(t) \equiv \begin{cases} \underset{\sim}{W}, & 0 \le t < 0.46 \\ 0.5\ \underset{\sim}{W} & 0.46 \le t < 1.22 \\ 0.25\underset{\sim}{W} & 1.22 \le t < 2.0 \end{cases} . \tag{6.62}$$

The resultant plot of $\sigma^2_{K+N}(\underset{\sim}{z}^*_K, z^*)$ as a function of time t_{K+N} is shown in Figure 6.31 where the effects of variable $\underset{\sim}{W}(t)$ in (6.62) are readily seen. As $\underset{\sim}{W}(t)$ decreases, so does the rate at which the uncertainty in the estimate of the maximum variance in the output grows. Thus, times between samples change greatly, changing the nature of the management problem. Though the plots of $[\underset{\sim}{P}^K_K(z_K)]_{11}$ are omitted for brevity, for reasons similar to those in the example of Section 6.3.4, the contours change from sample to sample affecting nonconstant solutions to the design problem.

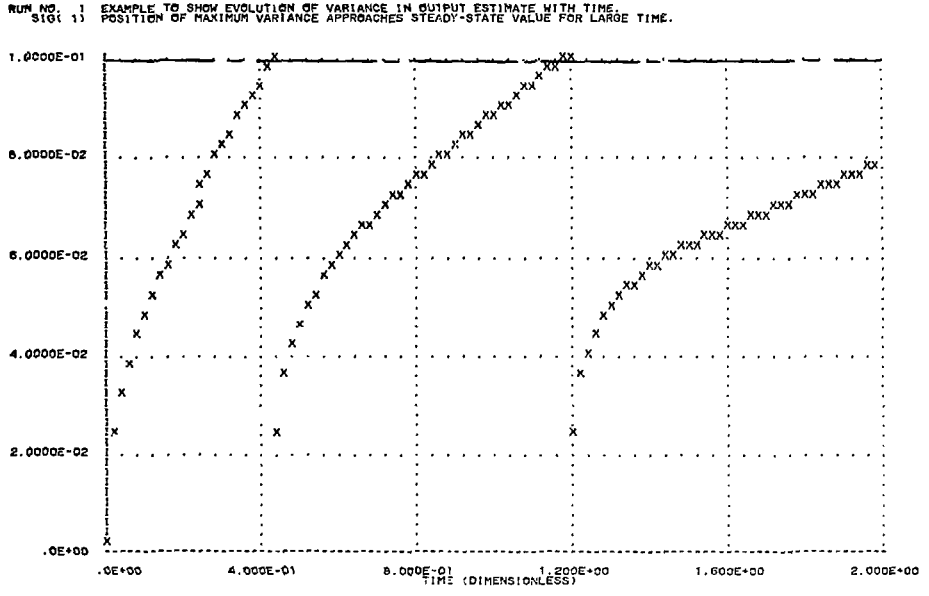


Figure 6.31. Time response of $\sigma^2_{K+N}\left(\underset{\sim}{z}^*_K, z^*\right)$ for time-varying disturbance statistics $\underset{\sim}{M}(t)$ given in (6.62).

Thus,

> Conclusion VIC. The solutions for the optimal monitoring design and management problems may not in general be the same for all measurement times if the disturbance noise statistics are allowed to vary with time. (C.VIC)

Second, fix the disturbance noise statistics $\underset{\sim}{W}$ to the value given in (6.61B) but now let the measurement error statistics vary from sample to sample. In this case, the sample times occur at t = 0.46, 0.80, 1.12, 1.38, 1.62, 1.80, and 1.94 over the interval $0 \leq t \leq 2$. Starting with $\underset{\sim}{V}$ given in (6.61C) for the first sample, let the measurement statistics be given by

$$\underset{\sim}{V}(t) \equiv \begin{cases} \underset{\sim}{V}, & t = 0.46 \\ 1.5\,\underset{\sim}{V}, & t = 0.80 \\ (1.5)^2\,\underset{\sim}{V}, & t = 1.12 \\ (1.5)^3\,\underset{\sim}{V}, & t = 1.38 \\ (1.5)^4\,\underset{\sim}{V}, & t = 1.62 \\ (1.5)^5\,\underset{\sim}{V}, & t = 1.80 \\ (1.5)^6\,\underset{\sim}{V}, & t = 1.94 \end{cases} \tag{6.63}$$

The plot of $\sigma^2_{K+N}(\underset{\sim}{z}^*_K, z^*)$ for $\underset{\sim}{V}(t)$ is shown in Figure 6.32. Note that $\underset{\sim}{V}(t)$ specified in (6.63) may be interpreted as taking consecutively worse and worse measurements from sample to sample. Thus, as the quality of the measurements decreases, the uncertainties in the estimate of the maximum variance in the output increase leading to higher initial conditions for the branches of σ^2_{K+N} after each measurement and resulting in shorter and shorter times between measurements. This completes the counterexamples for Conclusion VI which are summarized in

> Conclusion VID. The solutions for the optimal design and management problems may not in general be the same for all measurement times if the measurement error statistics at each sample are allowed to vary. (C.VID)

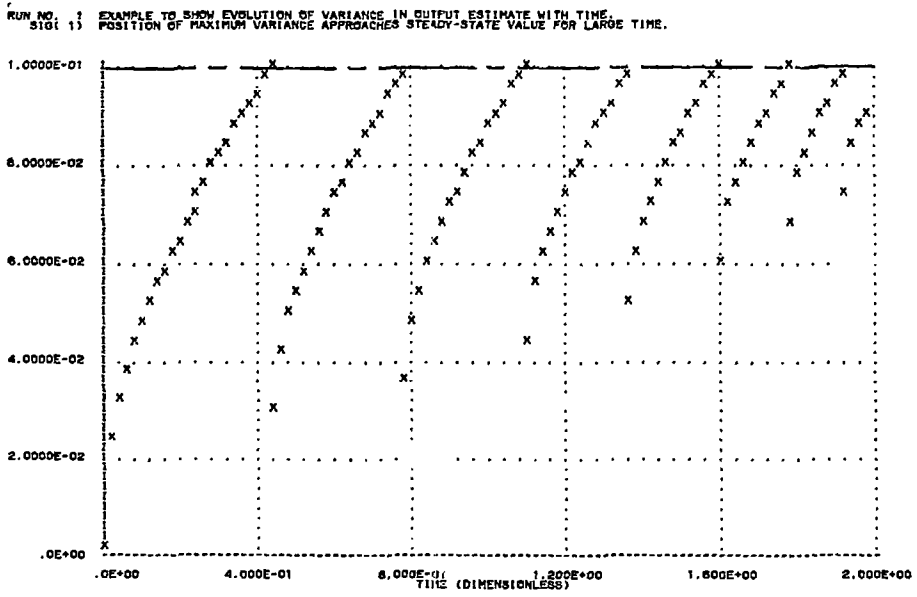


Figure 6.32. Time response of $\sigma^2_{K+N}\left(\underset{\sim}{\hat{z}}^*_K, z^*\right)$ for time-varying measurement statistics $\underset{\sim}{y}(t)$ given in (6.63).

6.3.8 Variable Number of Samplers — As shown in Section 5.3.4 and Conclusion VII, the optimum *number* of sampling devices to use at each measurement time t_K, the dimension m of the optimal measurement position vector $\underset{\sim}{z}_K^*$, is the same for every measurement in the infrequent sampling problem. In order to find that optimum number, the monitoring design problem is solved iteratively n times at the first measurement time t_K with $m = 1,2,\ldots, n$ samplers used in each iteration. This establishes a sequence of optimal measurement vectors $\underset{\sim}{z}_K^*$ of increasing dimension from which corresponding values of $[\underset{\sim}{P}_K^K(\underset{\sim}{z}_K^*)]_{11}$ may be found. To find the $\underset{\sim}{z}_K^*$ of optimal dimension, the various values of $[\underset{\sim}{P}_K^K(\underset{\sim}{z}_K^*)]_{11}$ are used to find the choice which leads to the fewest total number of samples necessary over the entire time interval of interest.

To demonstrate this concept, consider an example with $\sigma_{lim}^2 \equiv 0.1$, $\underset{\sim}{W} \equiv 0.125$, $\underset{\sim}{P}_0^0 \equiv \underset{\sim}{M}_0$ given in (6.57) and the measurement error in each measurement given by $[\underset{\sim}{V}]_{ii} = 0.05$, $i = 1,2,\ldots,m$. Since the number of modal states retained $n = 5$, five cases are compared with from one to five samplers used for each measurement in each case.

To find the optimum number of sensors m, for the case of bound on output error in the infrequent sampling problem, from Conclusion X, a measurement is necessary at time t_{K+N} when

$$\left[\underset{\sim}{P}_K^K(\underset{\sim}{z}_K^*)\right]_{11} + N[\underset{\sim}{\Omega}]_{11} + \underset{\sim}{c}(z^*)^T \underset{SS}{\Omega}\, \underset{\sim}{c}(z^*) \geq \sigma_{lim}^2, \qquad (6.64)$$

where the m-vector $\underset{\sim}{z}_K^*$ is the vector of optimal position locations and z^* from (5.72) is the position of maximum variance in the output $\sigma_{K+N}^2(\underset{\sim}{z}_K^*, z)$ over all positions z in the medium.

In order to compare the optimal $\underset{\sim}{z}_K^*$ for various dimensions m, first find

$$\underset{\sim}{g}(z^*)^T \underset{\sim}{\Omega}_{SS} \underset{\sim}{g}(z^*) \equiv \max_{z} \underset{\sim}{g}(z)^T \underset{\sim}{\Omega}_{SS} \underset{\sim}{g}(z). \tag{6.65}$$

This value is found by computation according to (5.72) where the matrix $\underset{\sim}{\Omega}_{SS}$ is defined in (5.20). For this problem, with the stochastic point source at $z_w \equiv 0.3$ and including $n \equiv 5$ modes in the model, the position of maximum variance

$$z^* = 0.2711. \tag{6.66}$$

Then, by computation,

$$\underset{\sim}{g}(z^*)^T \underset{\sim}{\Omega}_{SS} \underset{\sim}{g}(z^*) = 0.0417. \tag{6.67}$$

For the first measurement at time t_K, an expression for the time interval until the next sample is necessary can be obtained from (6.64) as follows. For this problem, the integration time step for $n \equiv 5$ for the time interval $0 \leq t < 1$ is chosen as

$$T \equiv \left(t_{K+1} - t_K\right) = 0.01. \tag{6.68}$$

The time to the next sample necessary is thus

$$\Delta t_{K+N} \equiv \left(t_{K+N} - t_K\right) = (N)(T), \tag{6.69}$$

where, from (6.64), the number of time steps

$$N = \frac{1}{[\underset{\sim}{\Omega}]_{11}} \left(\sigma^2_{lim} - \left[\underset{\sim}{P}^K_K(\underset{\sim}{z}^*_K)\right]_{11} - \underset{\sim}{g}(z^*)^T \underset{\sim}{\Omega}_{SS} \underset{\sim}{g}(z^*)\right). \tag{6.70}$$

The results starting at $t_0 \equiv 0$ with initial covariance matrix $\underset{\sim}{P}^0_0 \equiv \underset{\sim}{M}_0$ as in (6.57) led to the times of the first measurement $t_K = 0.46$. The numerical determination of the optimal measurement position vectors $\underset{\sim}{z}^*_K$ at t_K for $m = 1,2,3,4$, and 5, along with the corresponding values for $[\underset{\sim}{P}^K_K(\underset{\sim}{z}^*_K)]_{11}$ and the longest times to the next required measurements Δt_{K+N} are summarized in the following table.

m	1	2	3	4	5
$\underset{\sim}{z}_K^*$	$\begin{bmatrix}0.15196\end{bmatrix}$	$\begin{bmatrix}0.13866\\0.13866\end{bmatrix}$	$\begin{bmatrix}0.13399\\0.13398\\0.13398\end{bmatrix}$	$\begin{bmatrix}0.13160\\0.13160\\0.13160\\0.13160\end{bmatrix}$	$\begin{bmatrix}0.13016\\0.13016\\0.13016\\0.13016\\0.13016\end{bmatrix}$
$\left[P_{\underset{\sim}{z}_K}^K(\underset{\sim}{z}_K^*)\right]_{11}$	0.022194	0.014246	0.010707	0.008705	0.007417
Δt_{K+N}	0.29	0.35	0.38	0.39	0.40

(6.71)

Thus, as the number of measurement devices m deployed at the first measurement time increases, so does the time interval Δt_{K+N} before the next measurement is required. However, over the entire time interval of interest, the optimal choice can clearly be seen to use only one measurement device at each sample. To see this, consider Figure 6.33 where plots are presented together for $\sigma^2_{K+N}(\underset{\sim}{z}_K^*, z^*)$ as a function of time and for all five optimal choices of $\underset{\sim}{z}_K^*$ for dimensions $m = 1$ through 5 (plotted with "1", "2", ..,"5"). At the end of the time interval $0 \leq t < 1$, the total number of measurements necessary for each case are

m	1	2	3	4	5
Total Samples	2	4	6	8	10

Clearly taking only one sample at each measurement time is best.

To see this another way, compare the two extreme cases for $m = 1$ and $m = 5$ to determine the optimal dimension m for the measurement vector $\underset{\sim}{z}_K^*$. From the table in (6.71), for $m = 1$, $\Delta t_{K+N}\big|_1 = 0.29$. If this is compared with the case for $m = 5$, where $\Delta t_{K+N}\big|_5 = 0.40$, if only one measurement device ($m = 1$) is used over five measurement times, $5 * \Delta t_{K+N}\big|_1 = 1.45$ time units would be covered whereas five measurement

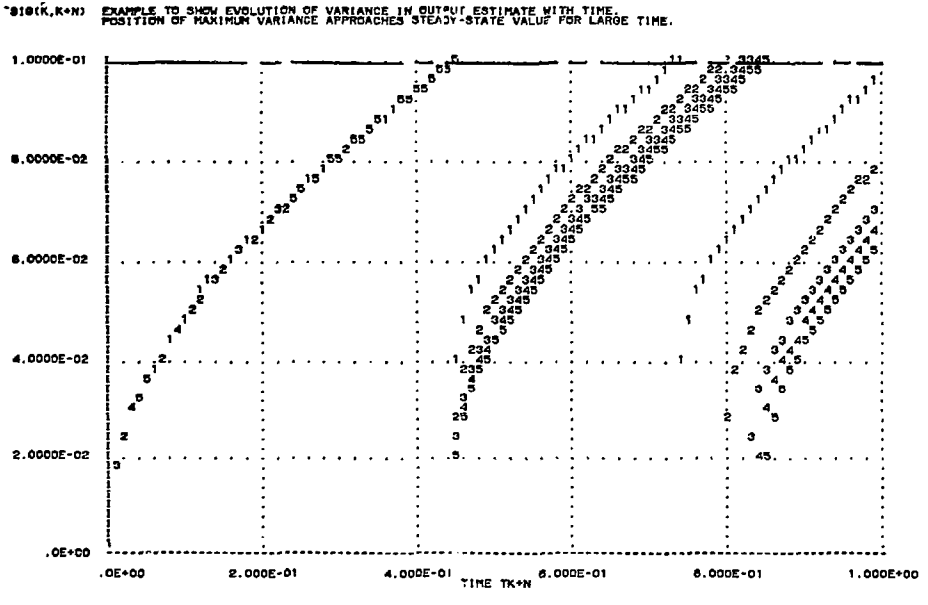


Figure 6.33. Time response of $\sigma^2_{K+N}\left(\underset{\sim}{z}^*_K, z^*\right)$ for optimal measurement position vectors $\underset{\sim}{z}^*_K$ of dimension m = 1, 2, 3, 4, and 5 plotted with corresponding symbols; note decrease in sampling frequency with number of measurements taken at each sample time.

devices used at only one measurement time results in $\Delta t_{K+N}\big|_5 = 0.40$. Both cases use a total of five samples but the case where only one sample is taken at each sample time leads to a much longer time interval overwhich the accuracy constraint is met.

Examination of the optimal measurement vectors $\underset{\sim}{z}_K^*$ in the table in (6.71) yields an observation regarding the placement of monitors of equal measurement quality which may be stated as

> Conjecture C. For the monitoring design problem using m statistically independent sampling devices of equal measurement quality at each measurement time, the optimal position of each sampling device is the same point in the medium. (C.C)

This is an interesting albeit obvious result which has arisen elsewhere for the steady-state solution of the Riccati equation associated with the continuous-time Kalman-Bucy Filter (see Hersch [56]). Its interpretation lies in the realization that since the measurement devices yield *uncorrelated* noise-corrupted measurements (that is, $\underset{\sim}{V}$ is assumed to be diagonal), the best position for one measurement device is also the best for all others. The optimal design, then, is to make m *statistically independent* samples all at the same point in the medium at each measurement time. This requirement of statistical independence has implications about actual hardware needed for each measurement; it would tend to rule out making more than one measurement with any given sensor at any one measurement time since the resultant additive noise would probably be correlated to some extent. This does, however, deserve closer study, and is not the point of this example.

6.3.9 Sensitivity of Results for the Infrequent Sampling Problem to Model Dimensionality — The effects of the size and complexity of the model of a physical process used in the analysis of any system upon the

results of that analysis is always a point of concern. Much work has been done elsewhere on related problems including a recent study of the quantitative simplification of normal mode models presented in Young [131], Chapter 2.

As mentioned earlier, it is not the intention of this study to explore this area in depth. However, a cursory look into model dimensionality as it relates to the infrequent sampling problem is in order here. Consider, then, the effects of increasing the dimension n of the normal mode model used in the Kalman Filter upon the results of optimal design and management problems for the case of infrequent sampling. As seen in previous examples, the variable of critical importance is the quantity $[\underset{\sim}{P}_K^K(\underset{\sim}{z}_K)]_{11}$; its minimization directly effects the optimal design and management problems and as will be seen in what follows, that minimization depends greatly upon the dimension of the model used in its calculation.

Consider a problem with bound on error in the output estimate with $\sigma^2_{z_{im}} \equiv 0.1$. Let the time interval of interest be $0 \leq t < 1$ with $\underset{\sim}{P}_0^0$, $\underset{\sim}{W}$, and $\underset{\sim}{V}$ given in (6.57), (6.20), and (6.21), respectively. Consider the sequence of problems with n = 5,6,7,8,9, and 10; the family of curves for $\sigma^2_{K+N}(\underset{\sim}{z}_K^*, z^*)$ is shown in Figure 6.34, plotted with symbols "5", "6", "7", "8", "9", and "Ø" for the same order. As can be seen immediately, the dimension of the Kalman Filter model can greatly effect the results in the optimal management problem.

To gain insight into the effect of the value of n upon the design problem, contour plots of $[\underset{\sim}{P}_K^K(\underset{\sim}{z}_K)]_{11}$ at the first sample for each case are shown in order in Figure 6.35. The addition of higher modes to the model is seen to complicate the nature of the $[\underset{\sim}{P}_K^K(\underset{\sim}{z}_K)]_{11}$-surface. This makes the optimization task for higher dimensional models more difficult

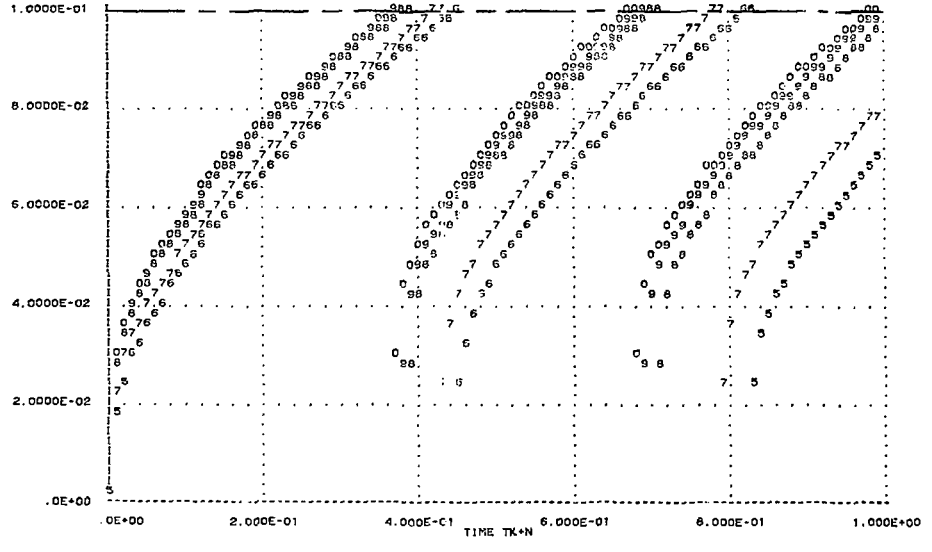


Figure 6.34. Time response of $\sigma^2_{K+N}\left(\underset{\sim}{z}^*_K, z^*\right)$ for filter models of dimension n = 5, 6, 7, 8, 9, and 10 plotted with corresponding symbols; note increase in sampling frequency with order of filter model.

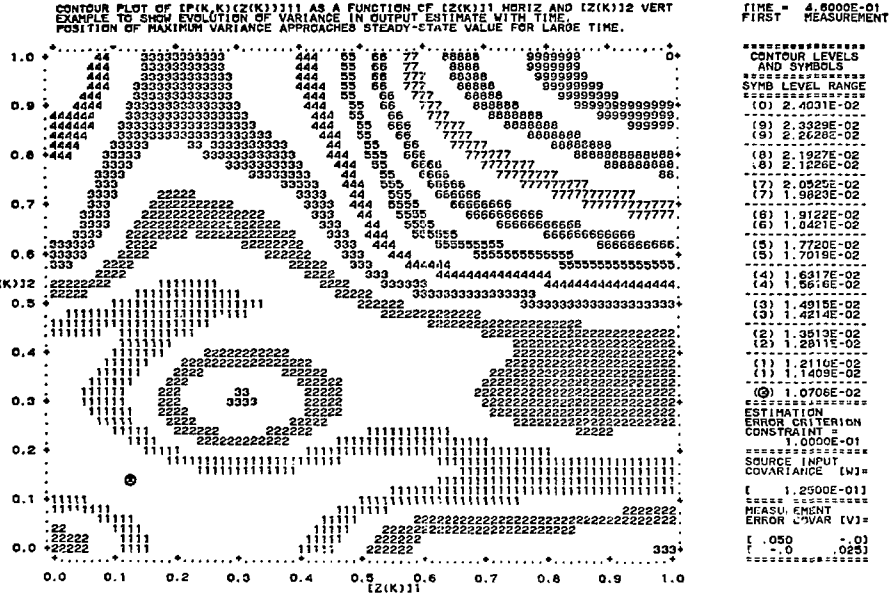


Figure 6.35A. Contour plot of $\left[P_K^K(\underset{\sim}{z}_K)\right]_{11}$ at first sample time $t_K = 0.46$ for filter model of dimension $n = 5$.

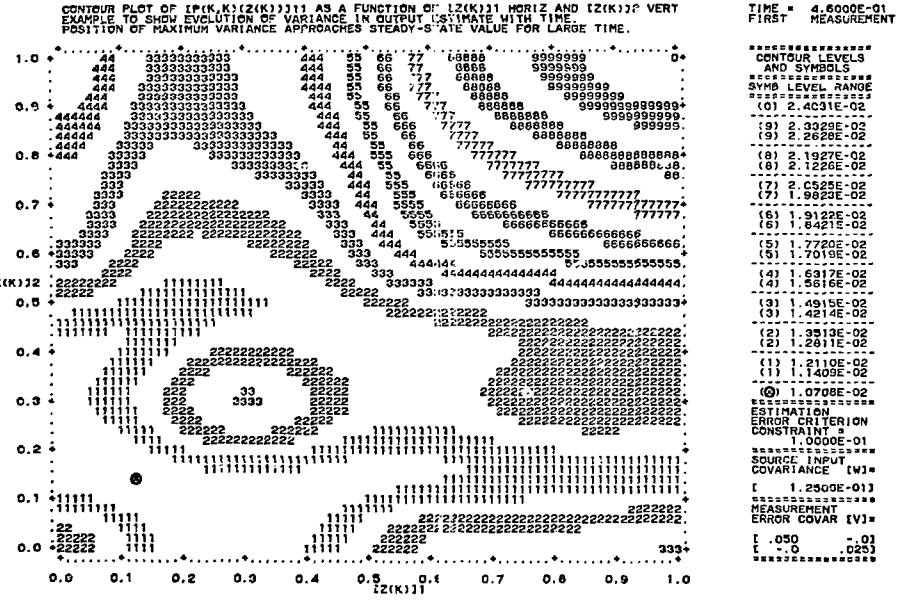


Figure 6.35B. Contour plot of $\left[P_K^K(\underline{z}_K)\right]_{11}$ at first sample time $t_K = 0.46$ for filter model of dimension $n = 6$; note similarity with case for $n = 5$ in Figure 6.35A.

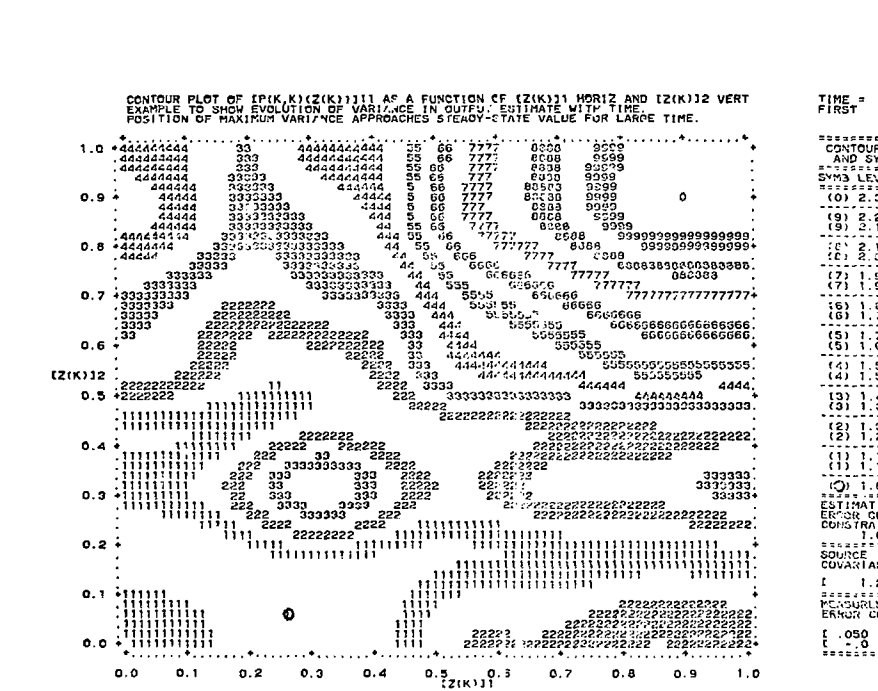


Figure 6.35C. Contour plot of $\left[P_{K|K}(z_K)\right]_{11}$ at first sample time $t_K = 0.44$ for filter model of dimension $n = 7$.

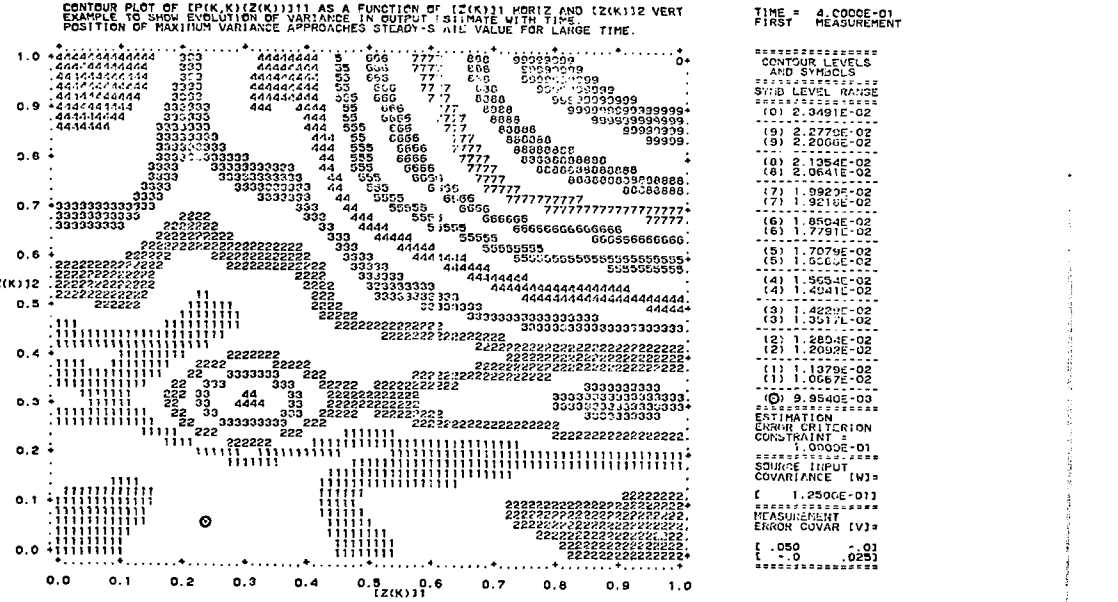


Figure 6.35D. Contour plot of $\left[\underline{P}_K^K(\underline{z}_K)\right]_{11}$ at first sample time $t_K = 0.40$ for filter model of dimension $n = 8$.

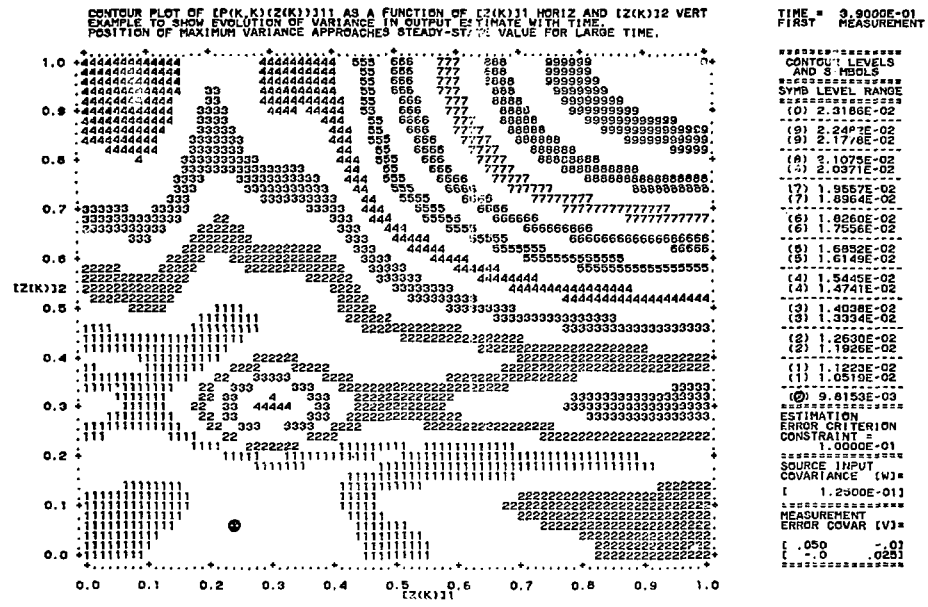


Figure 6.35E. Contour plot of $\left[P_{\underline{K}}^{K}(z_K)\right]_{11}$ at first sample time t_K = 0.39 for filter model dimension n = 9.

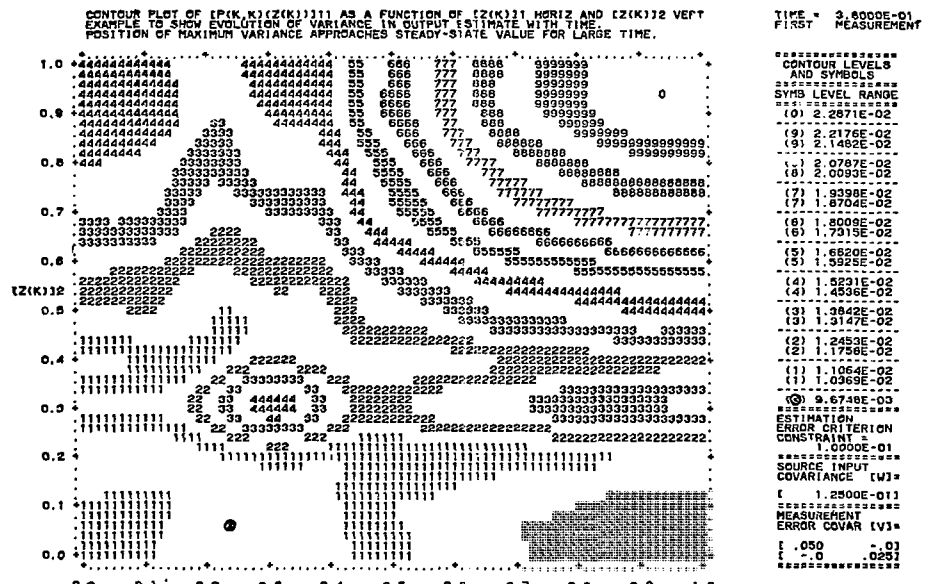


Figure 6.35F. Contour plot of $\left[P_K^K(\hat{z}_K)\right]_{11}$ at first sample time $t_K = 0.38$ for filter model of dimension $n = 10$.

owing to the addition of numerous local extrema. The classical approach to solving minimization problems which possess complicated objective functions is to increase the number of initial search points until sufficient confidence is obtained to suspect that the global minimum has been found; no other methods are known. Quoting from Beveridge and Schechter [20], p. 499, regarding finding the global optimum in a problem with multiple extrema

> "Thus, once a particular local minimum has been located by an appropriate search technique, it is important to check that other, better optima do not exist. There is no rigorous method for this search, except in certain restricted classes of problem. One can only begin the search procedure at a number of different initial base points."

Thus, the dimensionality of the filter model is seen to bear directly upon the complexity of the associated optimizations in the optimal design problem.

Another method of comparing the $[\underset{\sim}{P}_K^K(\underset{\sim}{z}_K)]_{11}$ surfaces for various model dimensions is by fixing one of the measurement positions and plotting sections through the surfaces over the range of dimensions for n as functions of the other measurement position. Such plots are included for values of $[\underset{\sim}{z}_K]_2 = 0.1$, 0.3, and 0.8. Schematically they represent cuts through the three-dimensional contour surfaces as in Figure 6.36. The three sets of curves for $n = 5$, 6,7,8,9, and 10 are shown in Figure 6.37. For the first two cuts, with $[\underset{\sim}{z}_K]_2 = 0.1$ and 0.3, large differences result particularly in the region of the source near $z_w \equiv 0.3$. For the third cut for $[\underset{\sim}{z}_K]_2 \equiv 0.8$, agreement is fairly good; note, however, that in contrast to the first cases, this cut is farther from the position of the source where it is seen that the effects of the source tend to be filtered out.

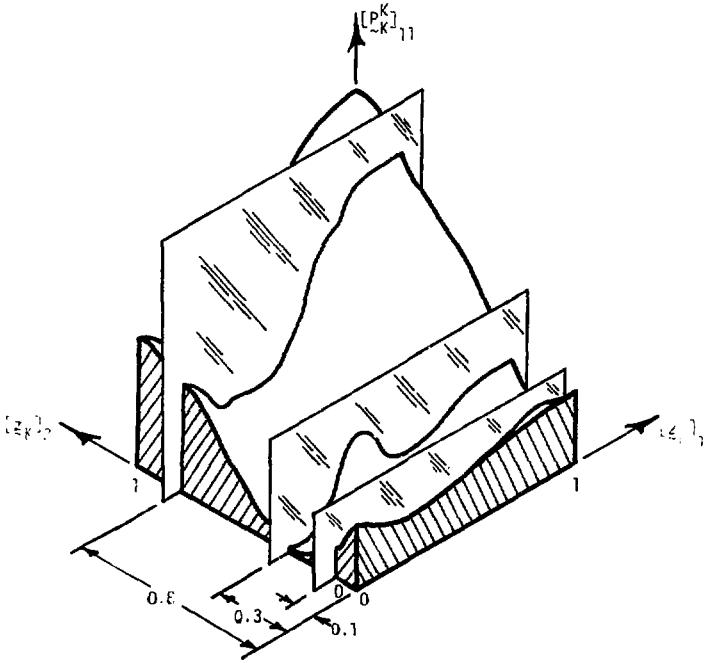


Figure 6.36. Schematic representation of the intersections of $[P^K_K(z_K)]_{11}$ surface with the planes $[z_K]_2 \equiv$ 0.1, 0.3, and 0.8.

Comparison of the contours in Figure 6.35 and particularly the cut for $[z_K]_2 = 0.1$ near the global minimima in $[P^K_K(z_K)]_{11}$ with the time responses for $\sigma^2_{K+N}(z^*_K, z^*)$ in Figure 6.37A gives rise to an apparent anomaly in the expected results; even though higher dimensional models in general are seen to result in *lower* optimal values for $[P^K_K(z^*_K)]_{11}$ at the sample times, the sampling *frequency* for higher dimensional models is greater. This can be explained as follows. Consider the situation

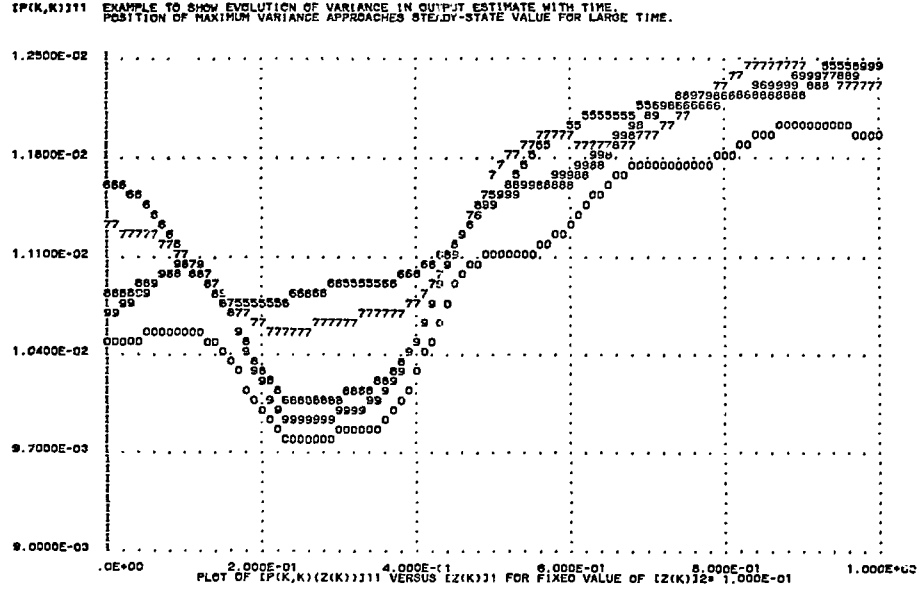


Figure 6.37A. Intersections of the $\left[P_{\underset{\sim}{K}}(\underset{\sim}{z}_K)\right]_{11}$ surfaces with the plane $\left[\underset{\sim}{z}_K\right]_2 \equiv 0.1$ plotted as functions of $\left[\underset{\sim}{z}_K\right]_1$ for filter models of dimension $n = 5,6,\ldots,10$ plotted with corresponding symbols.

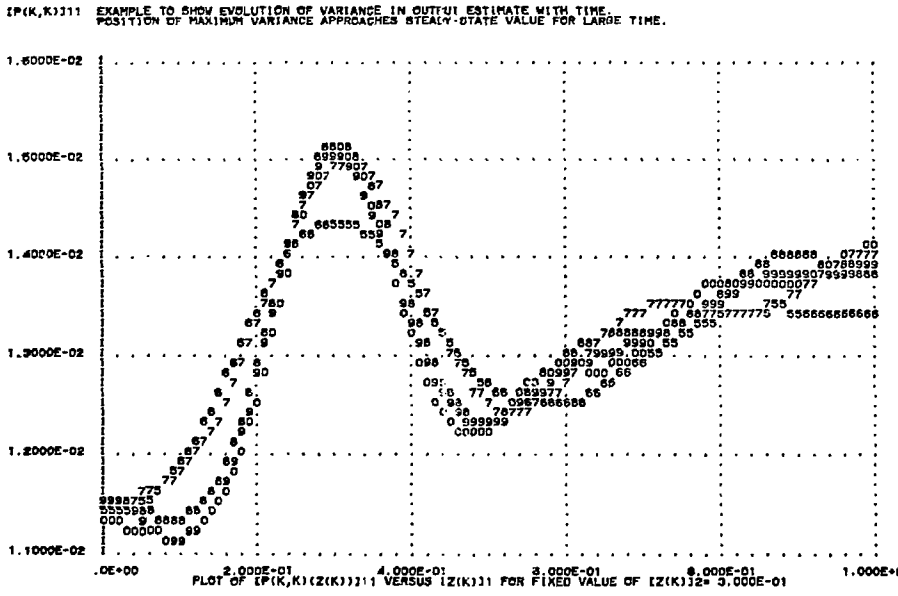


Figure 6.37B. Intersections of the $\left[P_K^K(z_K)\right]_{11}$ surfaces with the plane $\left[z_K\right]_2 \equiv 0.3$ plotted as functions of $\left[z_K\right]_1$ for filter models of dimension $n = 5,6,\ldots,10$, plotted with corresponding symbols.

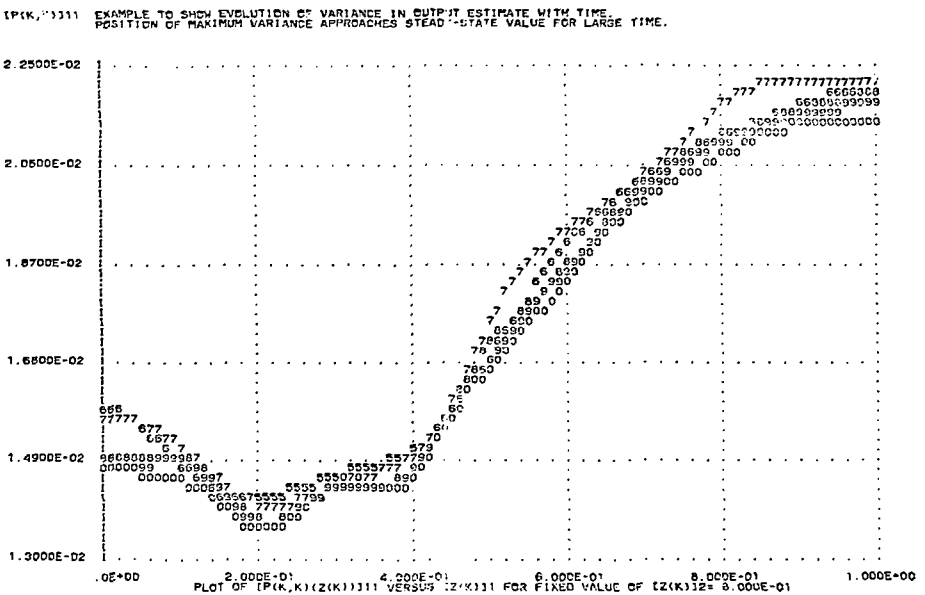


Figure 6.37C. Intersections of the $\left[P_{K}^{K}(z_K)\right]_{11}$ surfaces with the plane $\left[z_K\right]_2 \equiv 0.8$ plotted as functions of $\left[z_K\right]_1$ for filter models of dimension $n = 5,6,\ldots,10$, plotted with corresponding symbols.

at the first set of sample times. The results from the figures are summarized in the following table. Even though as n increases and

n	5	6	7	8	9	10
$\underset{\sim}{z}_K^*$	$\begin{bmatrix}0.1340\\0.1340\end{bmatrix}$	$\begin{bmatrix}0.1340\\0.1340\end{bmatrix}$	$\begin{bmatrix}0.2568\\0.0622\end{bmatrix}$	$\begin{bmatrix}0.2412\\0.0618\end{bmatrix}$	$\begin{bmatrix}0.2393\\0.0648\end{bmatrix}$	$\begin{bmatrix}0.2418\\0.0633\end{bmatrix}$
$\left[\underset{\sim}{P}_K^K(\underset{\sim}{z}_K^*)\right]_{11}$	0.010707	0.010707	0.010495	0.009953	0.009814	0.009674
$\sigma_K^2(\underset{\sim}{z}^*)$	0.02280	0.02280	0.02384	0.02697	0.02717	0.02828
t_K	0.460	0.460	0.440	0.400	0.390	0.380
$(t_{K+N} - t_K)$	0.380	0.380	0.360	0.320	0.310	0.310

(6.73)

$[\underset{\sim}{P}_K^K(\underset{\sim}{z}_K^*)]_{11}$ *decreases*, the time to the next sample, $(t_{K+N} - t_K)$, also *decreases*. Note however, that as n increases, so do the initial conditions on the trajectories for $\sigma_K^2(\underset{\sim}{z}_K^*, z^*)$. This effect stems from the fact that even though $[\underset{\sim}{P}_K^K(\underset{\sim}{z}_K^*)]_{11}$ gets smaller as n grows, more terms are being added into the quadratic forms for $\sigma_K^2(\underset{\sim}{z}_K^*, z^*)$ as the matrices increase in dimension.

The effect of this can be explained concisely in the asymptotic case for infrequent sampling by writing the expression for $\sigma_{K+N}^2(\underset{\sim}{z}_K^*, z^*)$ at the second set of sample times, t_{K+N}:

$$\sigma_{K+N}^2\left(\underset{\sim}{z}_K^*, z^*\right) \doteq \left[\underset{\sim}{P}_K^K\left(\underset{\sim}{z}_K^*\right)\right]_{11} + N[\underset{\sim}{Q}]_{11} + \underset{\sim}{c}(z^*)^T \underset{SS}{Q}\, \underset{\sim}{c}(z^*). \qquad (6.74)$$

As n increases, even though the term $[\underset{\sim}{P}_K^K(\underset{\sim}{z}_K^*)]_{11}$ decreases, the last term $\underset{\sim}{c}(z^*)^T \underset{SS}{Q}\, \underset{\sim}{c}(z^*)$ increases at a faster rate. Thus, for the same time period $(t_{K+N} - t_K)$, larger values of variance in the output result for models of larger dimension; thus, higher frequency sampling programs.

One final comparison is made for the monitoring problem with bound on error in the output estimate. The number of modal states retained in

the Kalman Filter model is seen to effect the outcome of the determinization of position of maximum variance in the output estimate. That is, the model dimension effects *where* in the medium the error in the pollutant estimate will first reach its limit. The maximization problem, restated, is:

> For time t_{K+N} given optimal measurement positions $\underset{\sim}{z}_K^*$ at time t_K, find z^* such that
>
> $$\sigma^2_{K+N}\left(\underset{\sim}{z}_K^*, z^*\right) = \max_{z} \sigma^2_{K+N}\left(\underset{\sim}{z}_K^*, z\right). \tag{6.75}$$

For the infrequent sampling problem in the case of no-flow boundary conditions, from Conclusion X, (6.75) was found to be equivalent to finding

$$\max_{z} \underset{\sim}{g}(z)^T \underset{\sim\sim}{\Omega}_{SS} \underset{\sim}{g}(z). \tag{6.76}$$

For the example treated here, plots of $\sigma^2_K(z)$ at the first sample times for the range of model dimensions n = 5 through 10 are shown in Figure 6.38. Results for the maximization problem are tabulated below.

n	5	6	7	8	9	10
z^*	0.2711	0.2711	0.2940	0.2922	0.2883	0.2957
$\underset{\sim}{g}(z^*)^T \underset{\sim\sim}{\Omega}_{SS} \underset{\sim}{g}(z^*)$	0.0417	0.0417	0.0447	0.0501	0.0509	0.0519

(6.77)

Recalling that the single point source is located at $z_w \equiv 0.3$, it is seen that as more modes are included in the model, the position of the maximum variance in the estimate of the output approaches the position of the source as expected; this is the point in the medium of greatest uncertainty in the estimate.

Notice that the steady-state term $\underset{\sim}{g}(z^*)^T \underset{\sim\sim}{\Omega}_{SS} \underset{\sim}{g}(z^*)$ does in fact increase with the dimension of the model n corroborating the reason

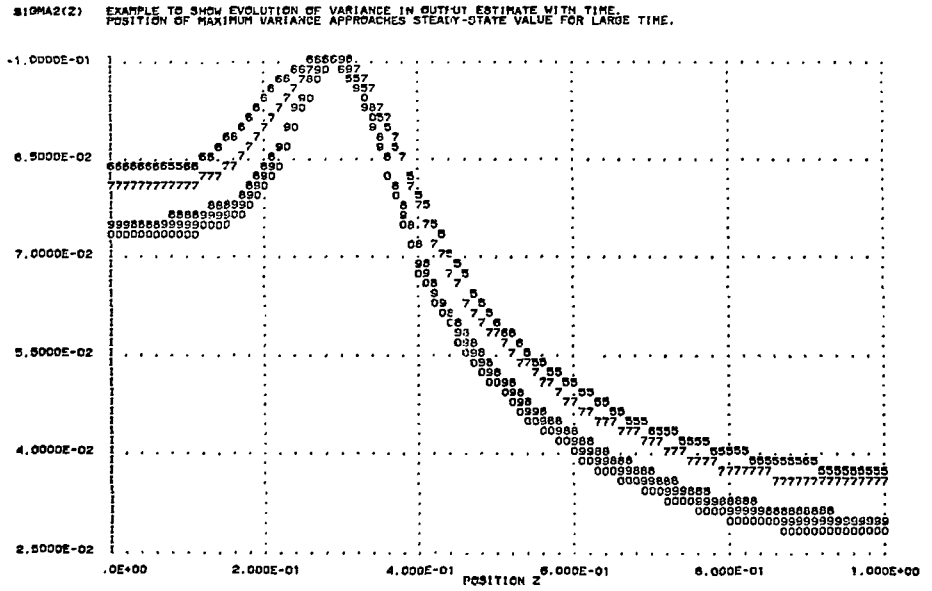


Figure 6.38. Plots of $\sigma_K^2(z_k^*, z^*)$ at first sample times t_K as functions of position z in the medium for filter models of dimension $n = 5,6,\ldots,10$ plotted with corresponding symbols.

behind the increased sampling frequencies for higher dimensional models.

Notice further in all of the data here that there are no differences for models of dimension $n = 5$ or 6. The reason for this can be seen by comparison of the input distribution matrices for the two models, the matrix $\underline{D}$ in equation (6.13). For these cases, computation yields

n	5	6
$\underline{D}$	1.000	1.000
	1.176	1.176
	-0.618	-0.618
	-1.902	-1.902
	-1.618	-1.618
		1.923×10^{-10}

(6.7b)

Thus, the contribution of the noise source to the sixth mode is seen to be negligible in comparison to the others. The reason for this is that the sixth mode characterized by its eigenfunction

$$e_6(z) = \cos(5\pi z)$$

possesses a zero at $z = 0.3$ which happens to be the location of the source. Thus, the addition of the sixth mode does not change the response of the model after its transient term has disappeared since that mode is unforced.

The results of this section are brought together in

> Conclusion XIX. The dimension of the model used in the optimal monitoring problem is seen to directly effect the results in the optimal design and management problems. (C.XIX)

A word of caution is in order then; in practical applications, tradeoffs are necessary as in all analyses involving finite dimensional models of infinite dimensional processes. Short of embarking upon a quantitative solution to the model simplification problem, the analyst

should assure himself that a model of a given dimension is sufficient to adequately represent his process. In the framework of the infrequent sampling problem, the mathematics associated with the sensitivity analysis of the results for the optimal monitor are seen to be particularly simple, providing a basis for rapid determination of adequate model complexity by straightforward comparison of numerical simulations.

6.3.10 Problems Including Pollutant Scavenging — All the examples thus far have been for the case of one-dimensional diffusion with no-flow boundary conditions and with no pollutant scavenging. Consider here cases where the scavenging term $-\alpha\zeta$ in the initial-boundary value problem (6.6) is nonzero. For the monitoring problem with bound on error in the output estimate, from Section 5.5.1, the maximum variance in the output estimate in the asymptotic case for infrequent sampling is given by

$$\sigma^2_{K+N}(\underset{\sim}{z}^*_K, z^*) = \left[\underset{\sim}{\rho}^K_K(\underset{\sim}{z}^*_K)\right]_{11} \phi_{11}^{2N} + [\Omega]_{11} \sum_{n=1}^{N} \phi_{11}^{2(n-1)} + \underset{\sim}{c}(z^*)^T \underset{SS}{\Omega}\, \underset{\sim}{c}(z^*). \tag{6.79}$$

From the state transition matrix $\underset{\sim}{\Phi}$ for the matrix $\underset{\sim}{A}$ in (6.13), it is seen that in (6.79),

$$\phi_{11} = \begin{cases} 0, & \alpha = 0 \\ e^{-\alpha T}, & \alpha \neq 0 \end{cases} . \tag{6.80}$$

Thus, the asymptotic growth of the first mode is a ramp of slope $[\Omega]_{11}$ for $\alpha = 0$ whereas it is a forced first-order response with a negative real eigenvalue for cases where $\alpha > 0$ in problems with scavenging. These differences are studied in the following examples.

Consider first the example of the previous section with $n = 5$ modal states. Choose for comparison the values $\alpha = 0$, 0.1, and 0.2. A plot of $\sigma^2_{K+N}(\underset{\sim}{z}^*_K, z^*)$ for the three cases using symbols "1", "2", and "3", respectively, is shown in Figure 6.39. For completeness, contour plots of $[\underset{\sim}{P}^K_K(\underset{\sim}{z}_K)]_{11}$ at the first sample times for the three values of α are shown in Figure 6.40. As suspected from the separation of variables in the eigenproblem of (5.83) and (5.84) in Section 5.5, the addition of scavenging has *no effect* upon the results for the optimal measurement design problem but does have a *direct effect* upon the management problem; the sampling frequency changes with α but the optimal measurement locations do not.

Consider a second example the cases $\alpha = 0$, 1, and 2; plots for these are included in Figure 6.41. It is seen that for both values of nonzero scavenging, no samples occurred within the interval $0 \leq t < 1$. From (5.20) it is found that the steady-state values of $\sigma^2_{K+N}(\underset{\sim}{z}^*_K, z^*)$ for the cases $\alpha = 1$ and 2 are as follows for the condition $0 < \phi_{11} < 1$:

From (5.18), the limit for the first term in (5.79) is

$$\lim_{N\to\infty} \left[\underset{\sim}{P}^K_K(\underset{\sim}{z}^*_K)\right]_{11} \phi^{2N}_{11} = 0; \tag{6.81A}$$

From (5.20) the limit for the second term in (5.79) is given by

$$\lim_{N\to\infty} [\underset{\sim}{\Omega}]_{11} \sum_{n=1}^{N} \phi^{2(n-1)}_{11} = \frac{[\underset{\sim}{\Omega}]_{11}}{1 - \phi^2_{11}}; \tag{6.81B}$$

Thus, by computation, obtain

α	1	2
$\lim_{N\to\infty}\left[\underline{P}_K^K(\underline{z}_K^*)\right]_{11}$	0	0
$\lim_{N\to\infty}[\underline{\Omega}]_{11}\sum_{n=1}^{N}\phi_{11}^{2(n-1)}$	0.06221	0.03124
$\underline{g}(z^*)^T\underset{SS}{\underline{\Omega}}\underline{g}(z^*)$	0.03782	0.03493
$\lim_{N\to\infty}\phi_{K+N}^2(\underline{z}_K^*,z^*)$	0.1000	0.06617

(6.81c)

For the case of $\alpha = 1$, the limiting value of $\sigma_{K+N}^2(\underline{z}_K^*,z^*)$ is seen to equal the estimation error limit $\sigma_{lim}^2 = 0.1$. Thus, this is seen to be the limiting case for the size of the scavenging term α for which the results of the infrequent sampling cease to apply; for values of $\alpha \geq 1$, no samples occur. For the case $\alpha = 2$, the limiting value for σ_{K+N}^2 is clearly below the estimation error limit.

It is seen, then, that for monitoring problems including scavenging, situations may arise in practice where a steady-state level of uncertainty in the pollutant estimate may exist which is below the specified estimation error limit. In these cases, it is never necessary to sample in order to assure that the estimation error remains below its limit; for such cases, the monitoring problem solution proposed here has no meaning.

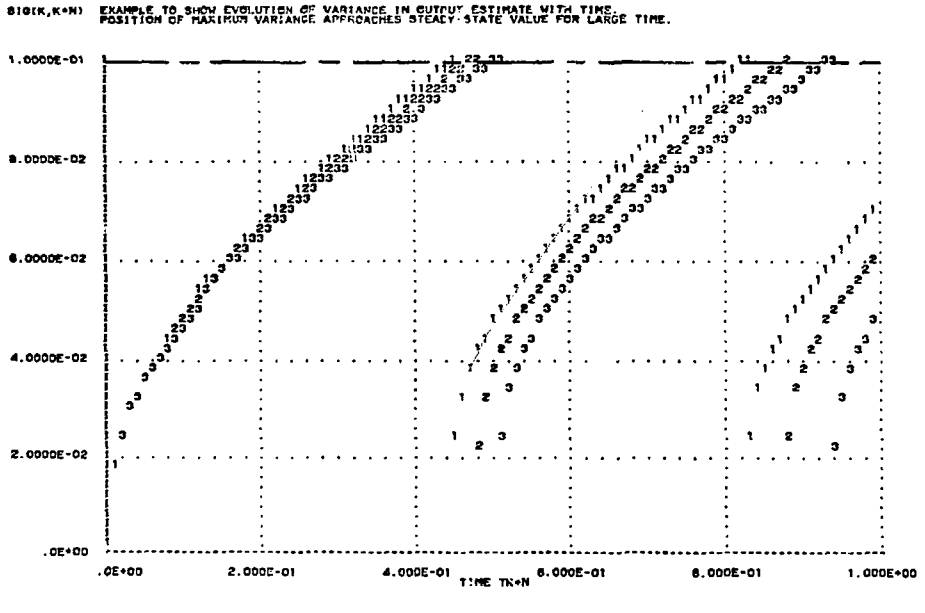


Figure 6.39. Plots of $\sigma^2_{K+N}\left(\underset{\sim}{z}^*_K, z^*\right)$ versus time t_{K+N} for systems with scavenging parameter $\alpha \equiv 0.0$, 0.1, and 0.2 plotted with symbols "1", "2", and "3", respectively.

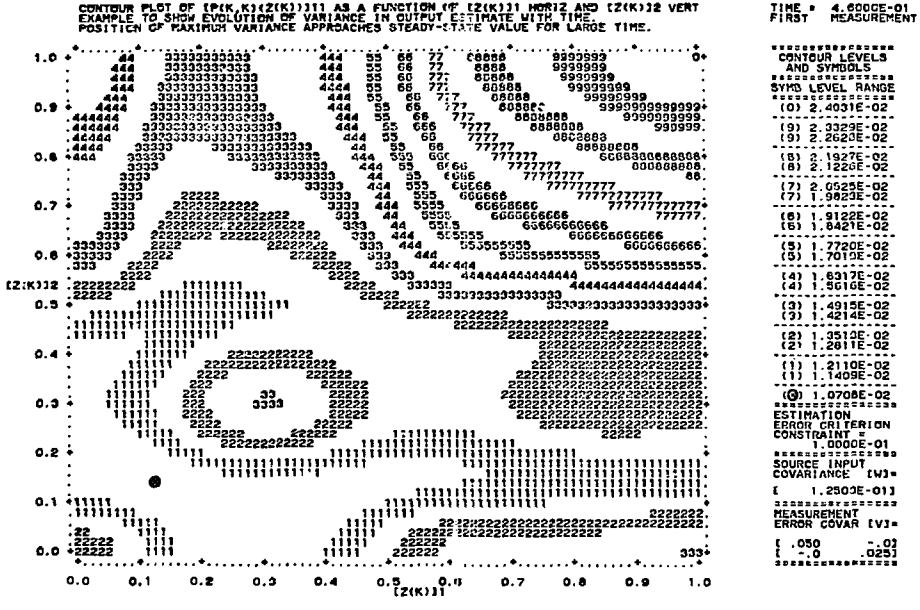


Figure 6.40A. Contour plot of $\left[P_K^K(z_K)\right]_{11}$ for the first sample at $t_K = 0.46$ for the case with scavenging parameter $\alpha \equiv 0.0$.

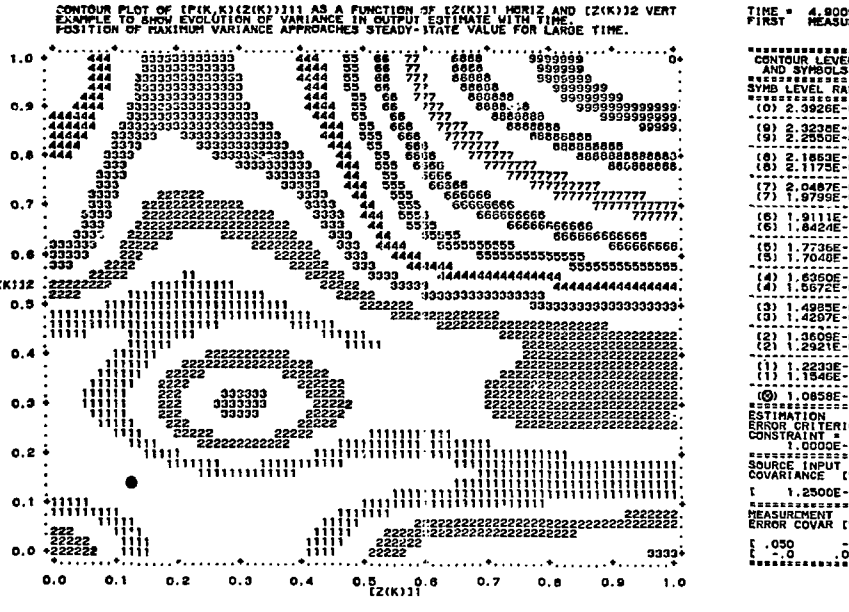


Figure 6.4[illegible]. Contour plot of $\left[P_K^K(z_K)\right]_{11}$ fo[illegible] the f[illegible] sample at $t_K = 0.49$ for the case with scavenging parameter $\alpha \equiv 0.1$.

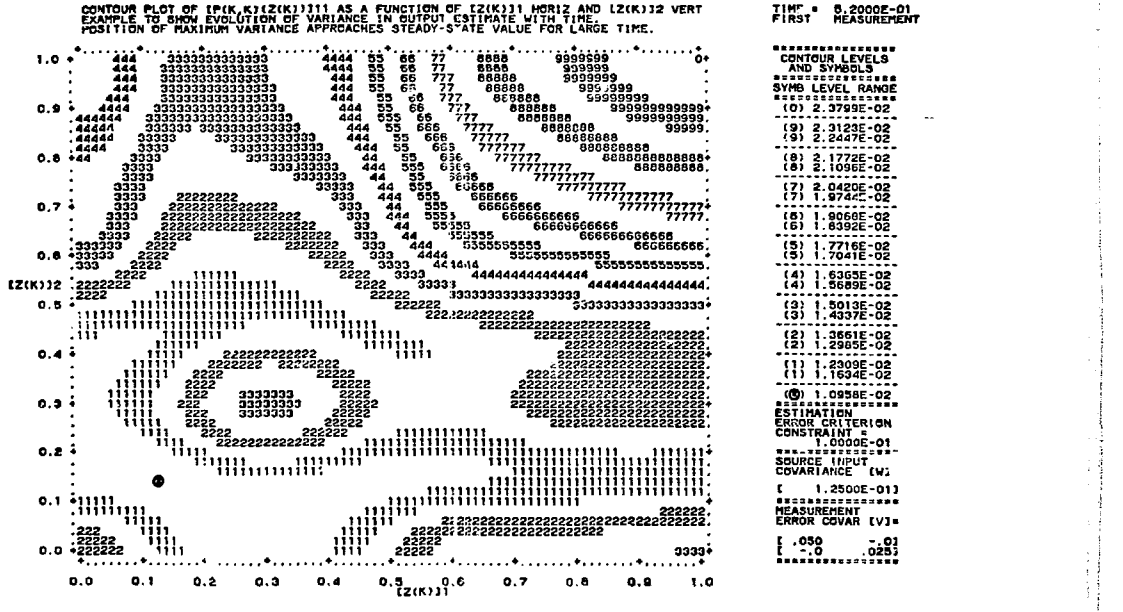


Figure 6.40C. Contour plot of $\left[\underline{P}_K^K(\underline{z}_K)\right]_{11}$ for the first sample at $t_K = 0.52$ for the case with scavenging parameter $\alpha \equiv 0.2$.

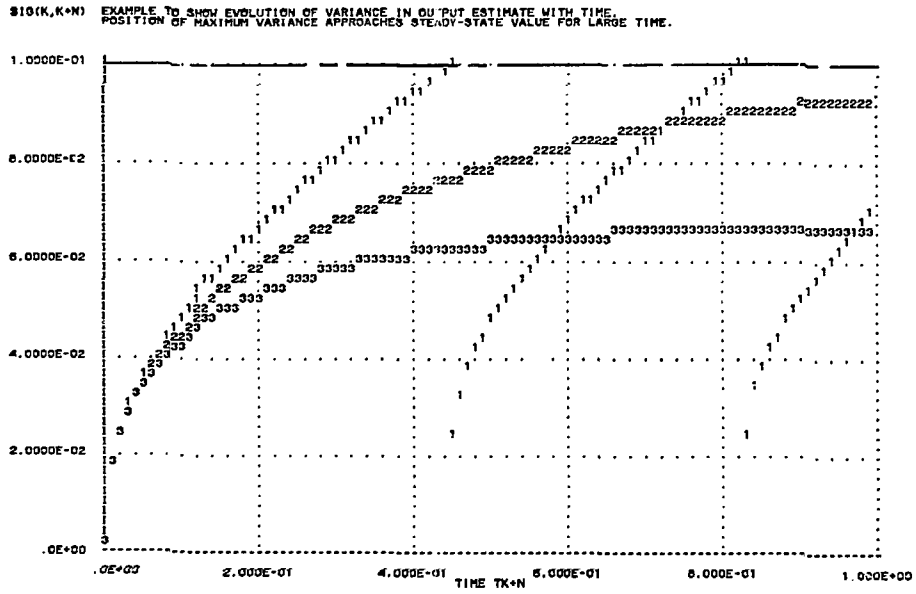


Figure 6.41. Plots of $\sigma^2_{K+N}\left(\underset{\sim}{z}^*_K, z^*\right)$ versus time t_{K+N} for systems with scavenging parameter $\alpha \equiv 0.0$, 1.0, and 2.0 plotted with symbols "1", "2", and "3", respectively. Notice how no samples occur for the cases with large scavenging terms; compare with Figure 6.39.

6.3.11. Problems with Multiple Sources — Though the results for the problem with a single point source are general, two cases are included here with multiple sources to demonstrate the applicability of the infrequent sampling concepts when more than one source is injecting pollutant into the medium. Compare three cases including one, two, and three point sources with their respective source location vectors given by

$$\underset{\sim}{z}_w \equiv \begin{bmatrix} 0.3 \end{bmatrix}, \qquad \underset{\sim}{z}_w \equiv \begin{bmatrix} 0.1 \\ 0.3 \end{bmatrix}, \qquad \underset{\sim}{z}_w \equiv \begin{bmatrix} 0.1 \\ 0.3 \\ 0.8 \end{bmatrix}. \tag{6.82}$$

For consistency, each of the three independent sources is specified by the same variance, $[\underline{W}]_{ii} \equiv 0.125$, $i = 1,2,3$, as in previous examples. Since the total disturbance to the system is more in the multiple source cases than for just one source as in past examples, the response of the output variance $\sigma^2_K(\underset{\sim}{z}^*_K, z^*)$ grows faster with time. In order to allow a sufficient number of time steps for the steady-state assumptions in (5.18) and (5.20) to hold, a larger error limit is used in these examples; $\sigma^2_{lim} \equiv 0.5$.

A plot of the maximum variance in the output estimate $\sigma^2_{K+N}(\underset{\sim}{z}^*_K, z^*)$ is included for the three cases in Figure 6.42; trajectories for one, two, and three sources are plotted with symbols "1", "2", and "3", respectively over the time interval $0 \leq t \leq 4$. It is seen that the greater the noise input to the total system, the faster the maximum uncertainty in the pollutant estimate increases.

Contour plots of $[\underset{\sim}{P}^K_K(\underset{\sim}{z}_K)]_{11}$ at the first sample times are shown for the cases with one, two, and three point sources in Figure 6.43. The general shapes of the surfaces change from those with just one source. For the two with multiple sources, the original source from all the

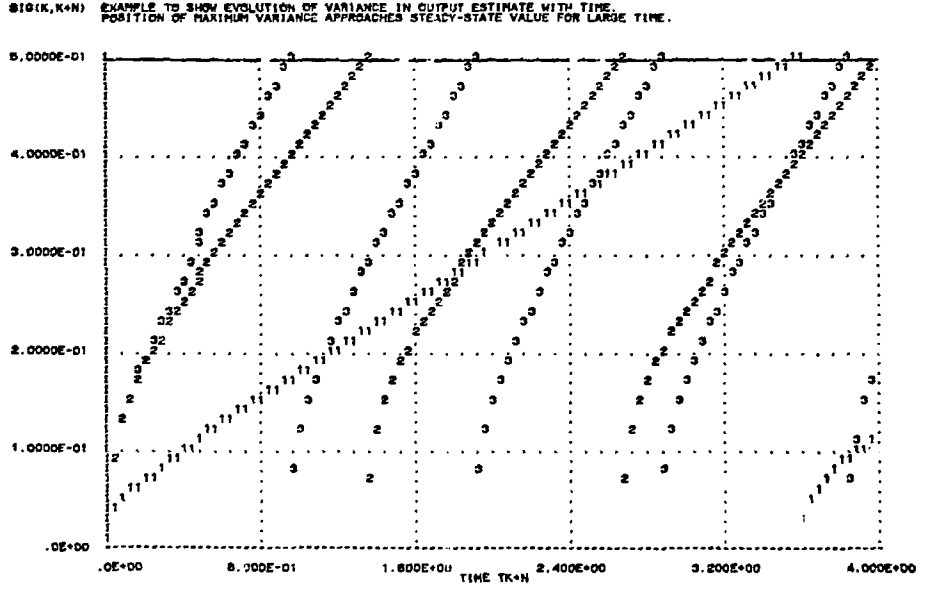


Figure 6.42. Plots of $\sigma^2_{K+N}(\underset{\sim}{z}^*_K, z^*)$ versus time t_{K+N} for systems with one, two, and three sources plotted with corresponding symbols, for sources with positions given in (6.82).

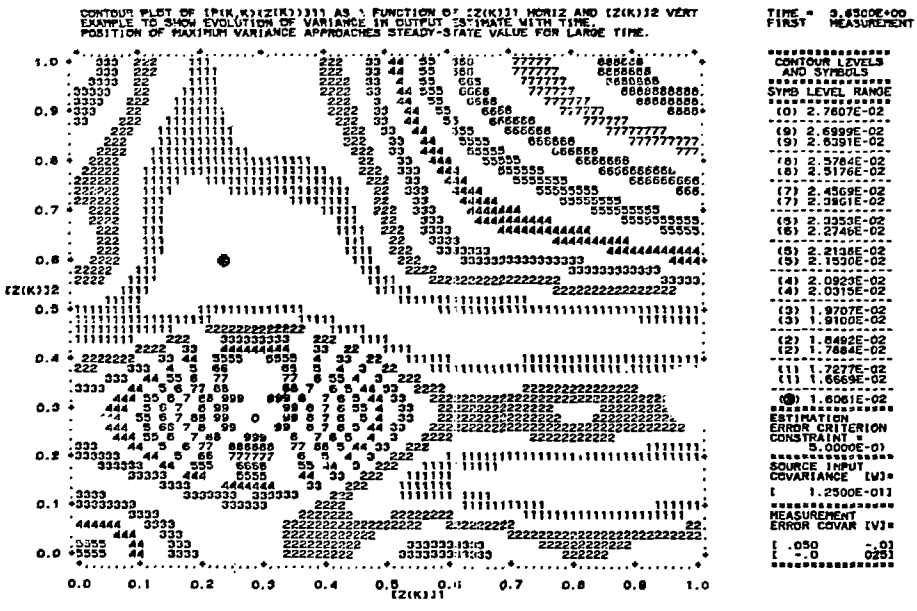


Figure 6.43A. Contour plot of $\left[P_K^K(z_K)\right]_{11}$ for the first sample at $t_K = 3.65$ for the case with one source at $z_w = 0.3$.

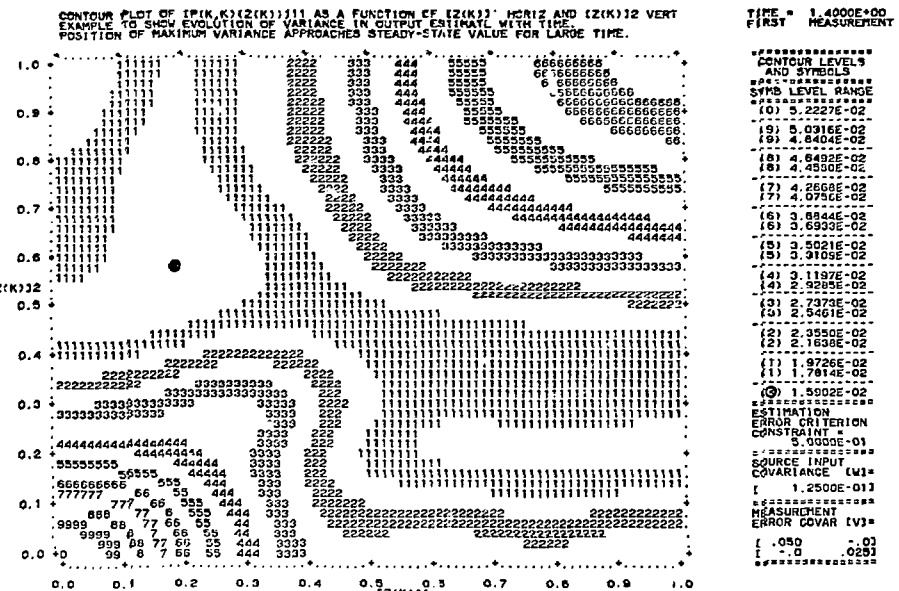


Figure 6.43B. Contour plot of $\left[P_K^K(z_K)\right]_{11}$ for the first sample at $t_K = 1.40$ for the case with two sources at $z_w \equiv [0.1, 0.3]^T$.

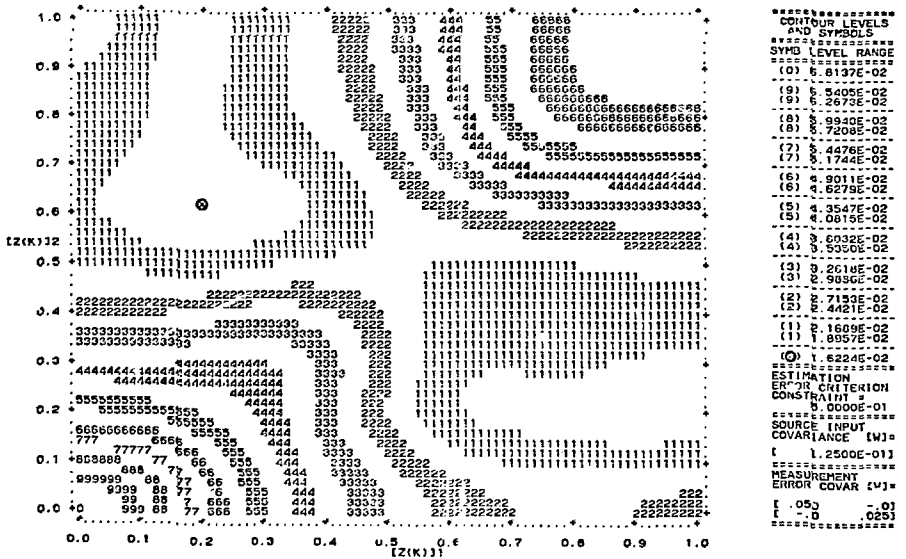


Figure 6.43C. Contour plot of $\left[P_K^K(z_K)\right]_{11}$ for the first sample $t_K = 1.00$ for the case with three sources at $\underline{z}_w \equiv [0.1, 0.3, 0.8]^T$.

previous examples is included at $z_w \equiv 0.3$ and results in the rises in the surfaces near that location. In Figure 6.34B, the second source at $z_w \equiv 0.1$ is added which significantly increases the uncertainty in the region near the left end of the medium. In Figure 6.43C, a third source at $z_w \equiv 0.8$ results in a slight rise in that area.

It seems in line with the results of Section 6.3.9 that the dimensionality of the model effects the sensitivity of the response of the surface $[P_K^K(z_K)]_{11}$ to the locations of sources in the medium. This can be explained as follows. The model used in these two cases has only five modes retained in the modal expansion. The spatial mode shape or eigenfunction for mode n is of the form $\cos((n-1)\pi z)$, where $0 \leq z \leq 1$ in these examples. Thus, near the end $z = 0$, all n modes have eigenfunctions which approach unity whereas for other positions out into the medium, cancellations can occur. Heuristically, the effect of a point source nearer $z = 0$, should be greater in each of the modal equations, resulting in a larger uncertainty in that region of the surface than in other areas. The response near $z_w \equiv 0.3$ and $z_w \equiv 0.8$ should then be more like that in the area of $z_w \equiv 0.1$ if a greater number of modes were retained. demonstrate this concept, Figure 6.44 shows the contour for $[P_K^K(z_K)]_{11}$ for the same problem with z_w as in (6.82) for three sources but with $n = 10$ modes retained. Comparing this plot with Figure 6.43C shows greater definition in the response near the region of the source at $z_w = 0.8$. In the limit, as $n \to \infty$, the response of the surface $[P_K^K(z_K)]_{11}$ to a single point source should be more nearly the same for all z_w, $0 \leq z_w \leq 1$.

In cases with multiple sources, the dimension of the model also effects the variance in the estimate of the output $\sigma^2_{K+N}(z_K^*, z)$ as a function

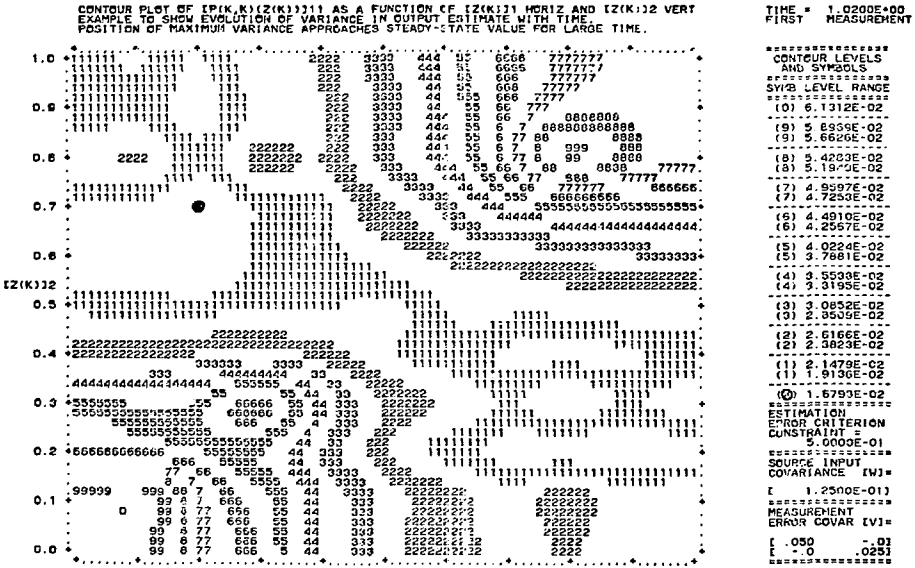


Figure 6.44. Contour plot of $\left[P_{K}^{K}(z_{K})\right]_{11}$ for the first sample at $t_K = 1.02$ for the case with three sources at $z_w \equiv [0.1, 0.3, 0.8]^T$, but with filter model of dimension $n = 10$. Compare with Figure 6.43C where $n = 5$; note higher resolution in surface near positions of three sources.

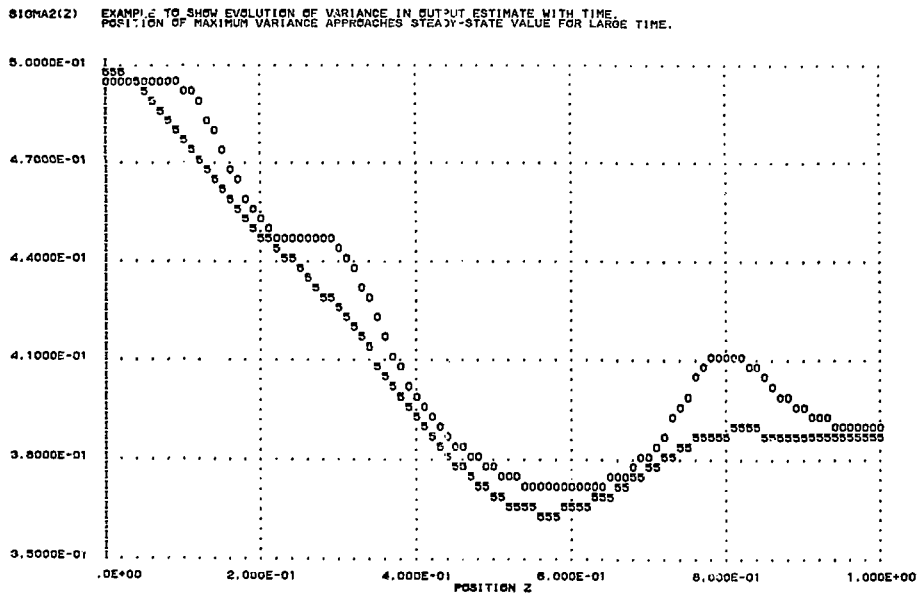


Figure 6.45. Plots of $\sigma^2_K(z^*_K, z)$ at first sample times t_K as functions of position z in the medium for case with three sources at $z_w \equiv [0.1, 0.3, 0.8]^T$ and filter models of dimension $n = 5$ and 10 plotted with symbols "5" and "0", respectively. Compare with cases with just one source at $z_w \equiv 0.3$ for models of various dimensions in Figure 6.38.

of position z in the medium. The cases corresponding to the plots of $[P_K^K(z_K)]_{11}$ in Figures 6.43C and 6.44 for $n = 5$ and 10 are plotted in Figure 6.45 with symbols "5" and "Ø", respectively. Here again, dimensionality effects the results.

6.4 Optimality in the Management Problem

Demonstration of the optimality of the monitoring sampling program as proposed in Section 5.8 can be made by cross-comparing many of the examples included above. Two particular choices from Section 6.3.5, perhaps, serve to demonstrate better than the others, extension of the scalar results of Conclusions XVI and XVII to the vector case. Let $\underset{\sim}{P}_0^0 \equiv \underset{\sim}{M}_0$ at t_0 be defined in (6.57) as before and choose the time interval of interest as $0 \leq t \leq 1$. Let $\sigma_{lim}^2 \equiv 0.150$ for a monitoring problem with bound on error in the output estimate. However, compare the following two sampling schedules:

(1) Predict to time t_{K_1} when

$$\sigma_{K_1}^2 \geq \left(\frac{5}{6}\right) \sigma_{lim}^2 = 0.125,$$

sample, then predict to $t = 1$;

(2) Predict to time t_{K_2} when

$$\sigma_{K_2}^2 \geq \sigma_{lim}^2 = 1.50,$$

sample, then predict to $t = 1$. (6.83)

The plot showing the trajectories for the two programs in (6.83) plotted with symbols "1" and "2", respectively is in Figure 6.46. Both schedules result in only one sample time over the interval $0 \leq t \leq 1$ such that, since both require the same number of samples to maintain the estimation error within its bound, the schedule resulting in the lower variance after both have sampled is clearly the better sampling program.

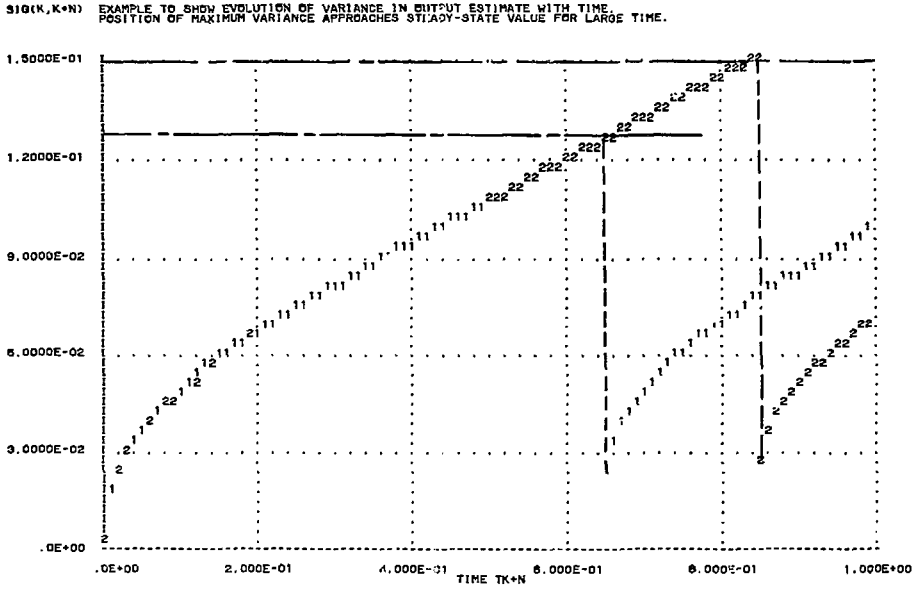


Figure 6.46. Plots of $\sigma^2_{K+N}\left(z^*_K, z^*\right)$ versus time t_{K+N} for sampling schedules (1) and (2) given in (6.38) plotted with corresponding symbols; note optimality of the second sampling program at end of time interval shown.

Since the error in schedule (2) is lower at the end of the interval, sampling at the limit, when at t_K, $\sigma_K^2 > \sigma_{lim}^2$ is seen to be superior. Thus, extension of the scalar results to this particular vector example shows that here sampling at the limit is optimal.

Naturally, this is not a proof but merely a demonstration in one particular example. However, for all cases studied to date, extension of the scalar results for the optimal management problem to the vector case has been seen to be valid, further indicating that proofs for the proposed extensions in Sections 5.8.2, 5.8.3, and 5.8.4 may be possible for the vector case.

CHAPTER 7. SUMMARY AND RECOMMENDED EXTENSIONS OF THE MAIN RESULTS

Here are gathered the main results for the class of optimal monitoring problem considered in this thesis with suggestions of certain areas in the theory where future expansions should be considered. The format is brief since concise statements of the conclusions resulting from this study, as listed at the beginning of this report, are contained within the main chapters themselves.

7.1 Summary

The problem of the optimal monitoring of pollutants in diffusive environmental media has been studied in the contexts of the subproblems of the optimal design and management of environmental monitors for bounds on maximum allowable errors in the estimate of the monitor state or output variables. Concise problem statements were made in Chapter 2; see (2.7) and (2.8). Continuous-time finite-dimensional normal mode models for distributed stochastic diffusive pollutant transport were developed in Chapter 3; see, for example, (3.37) and (3.40) and Figure 3.2. The resultant set of state equations was discretized in time for implementation in the Kalman Filter in the problem of optimal state estimation in Chapter 4; see the optimal filter algorithm summarized in Figure 4.1.

The theory of the solutions for problems of the optimal design and management of environmental monitoring systems was developed in Chapter 5. The general solution of the optimal monitoring problem with bound on error in the state estimate has been stated; see (5.13). The general solution for the optimal monitoring problem with bound on error in the output estimate has also been found; see (5.63).

The main results of this thesis concern the special class of optimal monitoring problem called the infrequent sampling problem. For the case of time-invariant linear stochastic diffusive systems, where the maximum errors allowable in the monitored estimates are relatively large, drastic simplifications in the solutions of the optimal monitoring design and management problems are possible as set forth in all of the conclusions in Chapters 5 and 6. The final results for the optimal monitoring design problem in the case of infrequent sampling with bound on error in the state estimate are contained in Conclusion VIII. The final results for the optimal monitoring design problem for the case of infrequent sampling with bound on error in the output estimate are contained in Conclusion XII. Extensions to systems including pollutant scavenging were made; results are in Conclusion XIII. Extensions were made to systems with fixed boundary conditions as summarized in Conclusion XIV. The theory was found to apply for systems with emission or radiation boundary conditions in Conclusion XV, which completed the extension in the design problem to all systems with general homogeneous boundary conditions.

The optimal management problem was solved analytically for scalar systems; see Conclusion XVII. Though an analytical result for the vector case of the optimal monitoring management problem was not found, an intuitively satisfying heuristic proof was proposed (see (5.196)) based upon the concept of the amount of correction made to the error in an estimate at a measurement in the scalar case found in Conclusion XVI.

The general result for the infrequent sampling monitoring problem in arbitrary coordinate systems with various boundary conditions is contained in Conclusion XVIII.

In Chapter 6, a considerable number of numerical examples are offered in substantiation of the theoretical results of Chapter 5. Various forms of graphical computer results serve to illustrate many of the more salient points of the theory of the infrequent sampling monitor.

7.2 Recommended Extensions

The main contribution of this study has been to demonstrate to future researchers that optimal solutions for monitoring problems in large, complex environmental systems will likely come from the study of an important special case: the infrequent sampling monitoring problem. A great number of extensions and refinements are seen possible by this author; this work has really only begun to scratch the surface of a large set of problems where the theory of the infrequent sampling problem may apply. Some of the more important areas for future consideration are suggested in what follows.

Recent extensions have been made by others of concepts of industrial engineering and operations research to the areas of dynamic system theory and optimal measurement system design. The work of Bar-Shalom, *et al.* [16] applies stochastic system theory to the resource allocation problem when uncertainty is included in the system. Aoki and Toda [5] have considered adaptive resource allocation for decentralized dynamic systems. All of these areas of theory — resource allocation as it applies to optimization of measurements, stochastic control as it relates to taking noise-corrupted measurements and decentralized dynamic systems for the study of large, coupled dynamic processes — are relavent areas for future study in the optimal environmental monitoring problem.

A useful extension of the fundamental concepts of Kalman Filter theory is to the problem of optimal pollutant surveillance in environmental

systems (see, for example, Brewer and Hubbard [23]). By using the smoothing form of the Kalman Filter (see Gelb [44], Bryson and Ho [26], and Jazwinski [65]), it is possible to construct a monitor whose purpose is to identify from measurement data the source which is injecting a harmful pollutant into an environmental region — its location, strength, etc. Such a detection/surveillance monitor could prove to be of great value to regional pollution control districts.

Many of the mathematical procedures used in this study are subject to refinement. Possibly the critical algorithm is that of the constrained optimization of a nonlinear function of many variables. The algorithm used here by Westley [127] was thought to be one of the superior gradient techniques in nonlinear programming when it was written. However, Westley [128] has since suggested consideration of the newer algorithms due to Abadie [1, 2], using the generalized reduced gradient method, as alternative and more powerful local minimization techniques. In this area of the extremization of a function with many local extrema, there is still the problem of determining whether or not the local minimum found is the *global* minimum. There still appears to be no analytical solution to the problem of global minimization [20]. Though not considered here, pure random search techniques, rather than steepest decent or gradient techniques, might possess better convergence characteristics for optimization in larger dimensional spaces which would result from any practical application in monitoring system synthesis; a starting point for future work here could be Kernopp [68].

The efficient and accurate modeling of environmental pollutant transport has long been a problem of concern to researchers and indeed continues to be. As the complexity and size of systems studied grows, so

does the need for more efficient modeling techniques. A new application of the collocation methods from the theory of partial differential equations has been made by Michelsen, *et al.* [94,124]; state-space models of extremely small dimension (like five or six states) have been used with greater accuracy than more routine finite-difference models of very large size (like one thousand cells) for the solution of the transport equations of a fixed-bed chemical reactor. This technique could be a powerful alternative to the separation of variables methods used in this study in systems where analytical expressions for eigensystems cannot be found, as was the case for fixed-bed reactors [39].

The general results for the infrequent sampling problem suggest potential application to any modeling technique for physical systems where certain dynamic terms dominate all others in the asymptotic response. This is allied to the theory of systems of stiff ordinary differential equations [43] and to the area of singular perturbations in control system design [72,131]. Application is thus seen to extend to mechanisms of pollutant dispersal other than just Fickian diffusion through the use of, say, finite-difference modeling techniques (see Goudreau [47] for comparisons of finite-difference methods). This is thought to be a particularly fertile area for future extensions, since by applying finite-difference techniques to distributed systems of various configurations, the resulting differential-difference equations could be cast into a form which can be diagonalized into a finite set of modal state equations (see Loscutoff [79]); these modal equations would then clearly exhibit the ordering of the eigenvalues which is essential to the infrequent monitoring problem.

Extensions are thus suggested to pollutant dispersal processes which combine diffusion with convection. Such processes embrace a wide variety of environmental systems, among them being air pollution, river and estuary water pollution and groundwater pollution. A recent study by Desalu, *et al.* [31] shows how stochastic models for air pollution can be derived, a way which lumps all the nondiffusive terms in the combined transport equation into time-varying source terms and then treats the resultant problem as one in Fickian diffusion. The use of such a technique seems to open a logical area for application of the theory associated with the infrequent sampling problem.

Other applications in such extensions to air pollution monitoring conceivably include use in the cost-optimal validation of regional and global atmospheric pollutant transport models [80,81]. Considerable effort is being made toward modeling regional atmospheric pollutant transport phenomena. Extension of the infrequent sampling ideas of this study to such areas could result in the cost-effective validation of such models. As mentioned before, application to modeling the upper atmosphere could help in determining where and when to fly high altitude aircraft for taking air samples for global atmospheric model validation. A likely application of the extension to surveillance monitoring systems mentioned above would be in detecting radon gas source positions and strengths in uranium mine shafts and in geothermal wells; the release of radon has been coming under closer scrutiny in recent years as man has increasingly disturbed the environments where it had heretofore remained entrapped.

Another application associated with uranium might be to the National Uranium Resource Evaluation Program. In this study, tens of thousands of soil samples are to be taken in the western United States. Upon determining the amounts of certain trace elements contained in these samples, this data will be used in a large pattern recognition computer program in order to learn whether the existence of such trace elements is correlated to uranium ore deposits in the areas where the samples were taken. An extension of the infrequent sampling ideas might include finding time scales over which dynamic models of the trace element transport through environmental systems would be valid. With the use of such models which would apply over, say, days, months, or years, cost-effective sampling programs for the identification of uranium deposits could result.

The initial application of optimal monitoring system synthesis concepts to river and estuary pollutant transport has been proposed by Moore [95]. This author feels that extensions of the infrequent sampling problem ideas could be made there to simplify monitoring system design for aquatic ecosystems.

Finally, applications could be studied in the areas of atomspheric and aquatic radiation monitoring systems. Applications are suggested in designing minimum-cost air sampling networks, for example, in the monitoring of atmospheric radiation levels in regions where underground nuclear experiments are conducted. An interesting extension of the surveillance application suggested above could be made here in attempting to identify sources of radiation from air samples gathered by a minimum-cost monitoring network. Another possible application could be to the cost-effective design of radiation detection networks for monitoring

groundwater radiation levels [120]. Variations of this might also include applications in the siting of nuclear power reactors and in the determination of best locations for their associated nuclear waste storage sites. In such applications, the intent would be to find locations where soil conditions were such that in the event of leakage of nuclear waste substances into the soil, effects to surrounding groundwater systems would be minimized.

All of these areas may be hypothetical at best but deserve future study, for the application and extension of the concepts presented in this study for the infequent sampling problem possess a great potential for improving and advancing the design procedures of cost-effective environmental pollution monitoring systems.

APPENDIX A. DISCRETIZATION OF THE STATE EQUATION

Given the linear, time-invariant system

$$\dot{\underset{\sim}{x}} = \underset{\sim}{A}\underset{\sim}{x} + \underset{\sim}{B}\underset{\sim}{u}, \tag{A.1}$$

Takahashi [121], and others have shown that for step size $T \equiv (t_{K+1} - t_K)$

$$\underset{\sim}{x}_{K+1} = e^{\underset{\sim}{A}T}\underset{\sim}{x}_K + e^{\underset{\sim}{A}T}\int_0^T e^{-\underset{\sim}{A}\tau}\,\underset{\sim}{B}\underset{\sim}{u}(\tau)\,d\tau, \tag{A.2}$$

$$\tau = t - KT.$$

This expression is now put into two more useable forms for machine application.

Since $\underset{\sim}{u}(t)$ is held constant over time intervals, i.e., $\underset{\sim}{u}(t) = \underset{\sim}{u}(t_K)$, $t_K \le t < t_{K+1}$,

$$\underset{\sim}{x}_{K+1} = e^{\underset{\sim}{A}T}\underset{\sim}{x}_K + e^{\underset{\sim}{A}T}\left[\int_0^T e^{-\underset{\sim}{A}\tau}\,d\tau\right]\underset{\sim}{B}\underset{\sim}{u}_K$$

$$= e^{\underset{\sim}{A}T}\underset{\sim}{x}_K + e^{\underset{\sim}{A}T}\left[-\underset{\sim}{A}^{-1}e^{-\underset{\sim}{A}\tau}\right]_0^T \underset{\sim}{B}\underset{\sim}{u}_K$$

$$= e^{\underset{\sim}{A}T}\underset{\sim}{x}_K + e^{\underset{\sim}{A}T}\left[-\left\{e^{-\underset{\sim}{A}T} - \underset{\sim}{I}\right\}\right]\underset{\sim}{A}^{-1}\,\underset{\sim}{B}\underset{\sim}{u}_K.$$

$$\Rightarrow \quad \underset{\sim}{x}_{K+1} = e^{\underset{\sim}{A}T}\underset{\sim}{x}_K + \left[e^{\underset{\sim}{A}T} - \underset{\sim}{I}\right]\underset{\sim}{A}^{-1}\,\underset{\sim}{B}\underset{\sim}{u}_K, \tag{A.3}$$

where the matrix exponential is given by

$$e^{\underset{\sim}{A}T} \equiv \sum_{n=0}^{\infty}\frac{(\underset{\sim}{A}T)^n}{n!} = \underset{\sim}{I} + \underset{\sim}{A}T + \frac{(\underset{\sim}{A}T)^2}{2!} + \ldots . \tag{A.4}$$

Equation (4.9) is verified with (A.3) and (A.4).

In cases where the system matrix $\underset{\sim}{A}$ is singular $\underset{\sim}{A}^{-1}$ does not exist and (A.3) cannot be used. Starting with (A.2), an alternative expression is sought for (A.3).

$$\underset{\sim}{x}_{K+1} = e^{\underset{\sim}{A}T}\underset{\sim}{x}_K + e^{\underset{\sim}{A}T}\left[\int_0^T e^{-\underset{\sim}{A}\tau}\, d\tau\right]\underset{\sim}{B}\underset{\sim}{u}_K \tag{A.2}$$

$$= e^{\underset{\sim}{A}T}\underset{\sim}{x}_K + \left[\int_0^T e^{\underset{\sim}{A}(T-\tau)}\, d\tau\right]\underset{\sim}{B}\underset{\sim}{u}_K.$$

$$\int_0^T e^{\underset{\sim}{A}(T-\tau)}\, d\tau = \int_0^T \left[\underset{\sim}{I} + \underset{\sim}{A}(T-\tau) + \frac{\underset{\sim}{A}^2(T-\tau)^2}{2!} + \ldots\right] d\tau$$

$$= \left[\underset{\sim}{I}\tau - \frac{\underset{\sim}{A}(T-\tau)^2}{2!} - \frac{\underset{\sim}{A}^2(T-\tau)^3}{3!} - \ldots\right]_0^T$$

$$= [\underset{\sim}{I}T] - \left[\underset{\sim}{0} - \frac{\underset{\sim}{A}T^2}{2!} - \frac{\underset{\sim}{A}^2T^3}{3!} - \ldots\right]$$

$$= \left[\underset{\sim}{I}T + \frac{\underset{\sim}{A}T^2}{2!} + \frac{\underset{\sim}{A}^2T^3}{3!} + \ldots\right] \tag{A.5}$$

$$\Rightarrow \underset{\sim}{x}_{K+1} = e^{\underset{\sim}{A}T}\underset{\sim}{x}_K + T\left[\underset{\sim}{I} + \frac{\underset{\sim}{A}T}{2!} + \frac{(\underset{\sim}{A}T)^2}{3!} + \ldots\right]\underset{\sim}{B}\underset{\sim}{u}_K. \tag{A.6}$$

Equations (4.10) and (4.11) are verified with (A.6).

APPENDIX B. DISCRETIZATION OF THE STATE DISTURBANCE STATISTICS

This Appendix details the development of a simple recursion for $\underline{\Omega}_{K+1}$ (see D'Appolito [29]), as outlined in Section 4.1.2.

Leibnitz's rule may be used to demonstrate that $\underline{\Omega}$ is a solution of a Riccati equation. Starting from the definition

$$\underline{\Omega}_{K+1} \equiv \underline{\Omega}(t)\Big|_{t=t_{K+1}} = \int_{t_K}^{t_{K+1}} \underline{\Phi}(t,\tau)\underline{D}\underline{W}(\tau)\underline{D}^T\underline{\Phi}(t,\tau)^T\, d\tau, \tag{4.14}$$

differentiate to get

$$\frac{d}{dt}\underline{\Omega}(t) = \int_{t_K}^{t} \left[\frac{\partial}{\partial t}\ \underline{\Phi}(t,\tau)\underline{D}\underline{W}(\tau)\underline{D}^T\underline{\Phi}(t,\tau)\right] d\tau$$

$$+ \underline{\Phi}(t,t)\underline{D}\underline{W}(t)\underline{D}^T\underline{\Phi}(t,t)^T\,\frac{d(t)}{dt}$$

$$- \underline{\Phi}(t,t_K)\underline{D}\underline{W}(t_K)\underline{D}^T\underline{\Phi}(t,t_K)^T\,\frac{d}{dt}\,(t_K)$$

$$= \int_{t_K}^{t} \left[\left(\frac{d}{dt}\underline{\Phi}(t,\tau)\right)\underline{D}\underline{W}(\tau)\underline{D}^T\underline{\Phi}(t,\tau)^T + \underline{\Phi}(t,\tau)\underline{D}\underline{W}(\tau)\underline{D}^T\left(\frac{d}{dt}\underline{\Phi}(t,\tau)\right)\right] d\tau$$

$$+ \underline{D}\underline{W}(t)\underline{D}^T$$

$$= \int_{t_K}^{t} \left[\underline{A}\underline{\Phi}(t,\tau)\underline{D}\underline{W}(\tau)\underline{D}^T\underline{\Phi}(t,\tau)^T\right] d\tau$$

$$+ \int_{t_K}^{t} \left[\underline{\Phi}(t,\tau)\underline{D}\underline{W}(\tau)\underline{D}^T\underline{\Phi}(t,\tau)^T\underline{A}^T\right] d\tau + \underline{D}\underline{W}(t)\underline{D}^T$$

$$= \underline{A} \int_{t_K}^{t} \underline{\Phi}(t,\tau)\underline{D}\underline{W}(\tau)\underline{D}^T\underline{\Phi}(t,\tau)^T \, d\tau$$

$$+ \left[\int_{t_K}^{t} \underline{\Phi}(t,\tau)\underline{D}\underline{W}(\tau)\underline{D}^T\underline{\Phi}(t,\tau)^T \, d\tau\right]\underline{A}^T + \underline{D}\underline{W}(t)\underline{D}^T \qquad (B.1)$$

or, finally,

$$\frac{d}{dt}\underline{\Omega}(t) = \underline{A}\underline{\Omega} + \underline{\Omega}\underline{A}^T + \underline{D}\underline{W}(t)\underline{D}^T; \; \underline{\Omega}(0) = \underline{0}. \qquad (B.2)$$

Since $\underline{\Omega}_{K+1}$ must satisfy the above matrix Riccati equation, matrix Riccati equation solution methods are sought for the evaluation of (4.14).

First, define the Hamiltonian H in terms of $\underline{x}$ and the costate vector $\underline{\xi}$ (see Kalman and Bucy [67] and Brewer [22]).

$$H \equiv -\frac{1}{2}\underline{x}^T\underline{D}\underline{W}\underline{D}^T\underline{x} - \underline{\xi}^T\underline{A}^T\underline{x}. \qquad (B.3)$$

From this, obtain Hamilton's equations

$$\frac{d\underline{x}}{dt} = \frac{\partial H}{\partial \underline{\xi}} = -\underline{A}^T\underline{x}$$

$$\frac{d\underline{\xi}}{dt} = -\frac{\partial H}{\partial \underline{x}} = \underline{D}\underline{W}\underline{D}^T\underline{x} + \underline{A}\underline{\xi}.$$

Adjoin the $\underline{x}$ and $\underline{\xi}$ vectors to obtain

$$\left[\begin{array}{c} \dot{\underline{x}} \\ \hline \dot{\underline{\xi}} \end{array}\right] = \left[\begin{array}{c|c} -\underline{A}^T & \underline{0} \\ \hline \underline{D}\underline{W}\underline{D}^T & \underline{A} \end{array}\right]\left[\begin{array}{c} \underline{x} \\ \hline \underline{\xi} \end{array}\right] \equiv \underline{A}\left[\begin{array}{c} \underline{x} \\ \hline \underline{\xi} \end{array}\right]. \qquad (B.4)$$

Define the $(2n \times 2n)$ state transition matrix $\underline{\Phi}$ for the system matrix $\underline{A}$ as

$$\Phi \equiv \left[\begin{array}{c|c} \Phi_{11} & \Phi_{12} \\ \hline \Phi_{21} & \Phi_{22} \end{array}\right] \tag{B.5}$$

where

$$\dot{\Phi} = A\Phi, \qquad \Phi(t,t) = I \tag{B.6}$$

Define $(n \times n)$ matrices χ and Θ such that

$$\left[\begin{array}{c} \dot{\chi} \\ \hline \dot{\Theta} \end{array}\right] = \left[\begin{array}{c|c} -A^T & Q \\ \hline DWD^T & A \end{array}\right] \left[\begin{array}{c} \chi \\ \hline \Theta \end{array}\right], \qquad \begin{array}{l} \chi(0) = I \\ \Theta(0) = \Omega(0) = Q. \end{array} \tag{B.7}$$

Make the equality

$$\Theta = \Omega\chi. \tag{B.8}$$

Differentiate to obtain

$$\dot{\Theta} = \dot{\Omega}\chi + \Omega\dot{\chi}. \tag{B.9}$$

Substitute from (B.7) to find

$$DWD^T\chi + A\Theta = \dot{\Omega}\chi - \Omega A^T\chi. \tag{B.10}$$

Since $\chi(0) = I$ and since χ is a state transition matrix, $\chi(t)^{-1}$ exists so that if

$$\Theta = \Omega\chi$$

then

$$\Theta\chi^{-1} = \Omega \tag{B.11}$$

and

$$\chi^{-1} = \Theta^{-1}\Omega. \tag{B.12}$$

Multiply (B.10) through by χ^{-1} and substitute (B.12) to get

$$\underline{D}\underline{W}\underline{D}^T + \underline{A}\underline{\Theta}\underline{\chi}^{-1} = \dot{\underline{\Omega}} - \underline{\Omega}\underline{A}^T$$

$$\Rightarrow \quad \dot{\underline{\Omega}} = \underline{A}\underline{\Omega} + \underline{\Omega}\underline{A}^T + \underline{D}\underline{W}\underline{D}^T. \tag{B.13}$$

Thus, by making the equality (B.8), it is seen that the solution of the matrix Hamilton's equations (B.7) is linked to the solution of the matrix Riccati equation (B.13).

The solution $\underline{\Omega}(t)$ of (B.12) can now be found. The solution of the Hamilton's equations (B.7) may be written

$$\begin{bmatrix} \underline{\chi}(t) \\ \hline \underline{\varrho}(t) \end{bmatrix} = \begin{bmatrix} \underline{\chi}(0) \\ \hline \underline{\varrho}(0) \end{bmatrix} + \begin{bmatrix} \underline{\Phi}_{11} & \underline{\Phi}_{12} \\ \hline \underline{\Phi}_{21} & \underline{\Phi}_{22} \end{bmatrix} \begin{bmatrix} \underline{I} \\ \hline \underline{0} \end{bmatrix}. \tag{B.14}$$

Thus, $\underline{\chi}(t) = \underline{\Phi}_{11}(t)$, $\underline{\varrho}(t) = \underline{\Phi}_{21}(t)$ and

$$\underline{\Omega}(t) = \underline{\Phi}_{21}(t)\underline{\Phi}_{11}(t)^{-1}. \tag{B.15}$$

From the form of $\underline{A}$ in (B.4),

$$\underline{\Phi}_{12} \equiv \underline{0}. \tag{B.16}$$

With this observation and using (B.6), it is found that

$$\dot{\underline{\Phi}}_{11} = -\underline{A}^T\underline{\Phi}_{11}, \qquad \underline{\Phi}_{11}(t_K,t_K) = \underline{I} \tag{B.17}$$

$$\dot{\underline{\Phi}}_{22} = \underline{A}\underline{\Phi}_{22}, \qquad \underline{\Phi}_{22}(t_K,t_K) = \underline{I} \tag{B.18}$$

$$\dot{\underline{\Phi}}_{21} = \underline{D}\underline{W}\underline{D}^T\underline{\Phi}_{11} + \underline{A}\underline{\Phi}_{22}, \qquad \underline{\Phi}_{21}(t_K,t_K) = \underline{0}. \tag{B.19}$$

From (B.17) and (B.18) for $T \equiv (t_{K+1} - t_K)$,

$$\underline{\Phi}_{11} = \underline{e}^{-\underline{A}^T T} \tag{B.20}$$

$$\underline{\Phi}_{22} = e^{\underline{A}T} \tag{B.21}$$

so that

$$\underset{\sim}{\Phi}_{11}^{-1} = \underset{\sim}{\Phi}_{22}^{T}. \tag{B.22}$$

Since

$$\underset{\sim}{\Phi}_{11}^{-1} = \left[e^{-\underset{\sim}{A}T}\right]^{-1} \tag{B.23}$$

and

$$\underset{\sim}{\Phi}_{22}^{T} = \left[e^{\underset{\sim}{A}T}\right]^{T}, \tag{B.24}$$

it is seen that

$$\underset{\sim}{\Phi}_{11}^{-1}\underset{\sim}{\Phi}_{11} = \underset{\sim}{I} = \underset{\sim}{\Phi}_{22}^{T}\underset{\sim}{\Phi}_{11} = \left[e^{\underset{\sim}{A}T}\right]^{T} e^{-\underset{\sim}{A}^{T}T} = \underset{\sim}{I}. \tag{B.25}$$

Thus, it has been verified that since (B.18) is the adjoint of (B.17),

$$\underset{\sim}{\Phi}_{11}^{-1} = \underset{\sim}{\Phi}_{22}^{T}. \tag{B.26}$$

This eliminated having to use an inverse, resulting in the equation sought for $\underset{\sim}{\Omega}$,

$$\underset{\sim}{\Omega} = \underset{\sim}{\Phi}_{21}\underset{\sim}{\Phi}_{22}^{T}. \tag{B.27}$$

Thus, the problem of finding $\underset{\sim}{\Omega}$ reduces from solving a matrix Riccati equation to solving for two state transition matrices, $\underset{\sim}{\Phi}_{21}$ and $\underset{\sim}{\Phi}_{22}$.

The computational algorithm for finding $\underset{\sim}{\Omega}$ is now developed. The system under study is time-invariant with calculational step size $T \equiv (t_{K+1} - t_K)$ so that

$$\underset{\sim}{\Phi}(t_{K+1} - t_K) = \underset{\sim}{\Phi}(T) = \sum_{n=0}^{\infty} \frac{(\underset{\sim}{A}T)^n}{n!}. \tag{B.28}$$

From (B.17) and (B.18),

$$\underline{\Phi}_{11}(T) = \sum_{n=0}^{\infty} \frac{(\underline{A}^T T)^n}{n!} \tag{B.29}$$

$$\underline{\Phi}_{22}(T) = \sum_{n=0}^{\infty} \frac{(\underline{A}T)^n}{n!} . \tag{B.30}$$

Since $\underline{\Phi}_{12}(T) = \underline{0}$, $(\underline{A}T)^n$ must have the form

$$(\underline{A}T)^n = \left[\begin{array}{c|c} (-\underline{A}^T T)^n & \underline{0} \\ \hline \underline{F}_n & (\underline{A}T)^n \end{array}\right]. \tag{B.31}$$

An expression is sought for $\underline{F}_n$ to be used in computing $\underline{\Phi}_{21}$. In order to obtain a recursive relationship for $\underline{F}_n$, right multiply $(\underline{A}T)^n$ by $(\underline{A}T)$,

$$\left[\begin{array}{c|c} (-\underline{A}^T T)^n & \underline{0} \\ \hline \underline{F}_n & (\underline{A}T)^n \end{array}\right]\left[\begin{array}{c|c} (-\underline{A}^T T) & \underline{0} \\ \hline \underline{D}\underline{W}\underline{D}^T T & \underline{A}T \end{array}\right] = \left[\begin{array}{c|c} (-\underline{A}^T T)^{n+1} & \underline{0} \\ \hline -\underline{F}_n(\underline{A}^T T) + (\underline{A}T)^n \underline{D}\underline{W}\underline{D}^T T & (\underline{A}T)^{n+1} \end{array}\right] \tag{B.32}$$

From which,

$$\underline{F}_{n+1} = (\underline{A}T)^n \underline{D}\underline{W}\underline{D}^T T - \underline{F}_n(\underline{A}^T T), \qquad \underline{F}_0 = \underline{0}. \tag{B.33}$$

Define

$$\tilde{\underline{F}}_n = \frac{\underline{F}_n}{n!}, \qquad \tilde{\underline{A}}_n = \frac{(\underline{A}T)^n}{n!} . \tag{B.34}$$

Thus, the algorithm equations are

$$\tilde{\underline{F}}_{n+1} = \frac{1}{n+1}\left[\tilde{\underline{A}}_n \underline{D}\underline{W}\underline{D}^T T - \tilde{\underline{F}}_n(\underline{A}^T T)\right], \qquad \tilde{\underline{F}}_0 \equiv \underline{0}, \tag{B.35}$$

$$\tilde{\underline{A}}_{n+1} = \frac{\underline{A}T}{n+1}\tilde{\underline{A}}_n, \qquad \tilde{\underline{A}}_0 \equiv \underline{I}, \tag{B.36}$$

$$\underset{\sim}{\Phi}_{21}(T) \cong \sum_{n=0}^{k} \tilde{\underset{\sim}{F}}_n, \tag{B.37}$$

$$\underset{\sim}{\Phi}_{22}(T) = \sum_{n=0}^{k} \tilde{\underset{\sim}{A}}_n. \tag{B.38}$$

Here, k is the number of terms necessary to adequately approximate the infinite series expressions. In practice, it is found using a method due to Paynter (see Brewer [22]).

$$\underset{\sim}{\Omega}_{K+1} \equiv \underset{\sim}{\Omega}(T) = \underset{\sim}{\Phi}_{21}(T)\underset{\sim}{\Phi}_{22}^{T}(T), \qquad T \equiv (t_{K+1} - t_K). \tag{B.39}$$

Thus, the discretized form of the state disturbance covariance matrix convolution (4.26) has been shown as the product of two state transition matrices, obtainable with the algorithm (B.35) - (B.39).

APPENDIX C. STATE AND ERROR COVARIANCE PREDICTION WITHOUT MEASUREMENTS

In this Appendix are developed relationships useful to the monitor management problem for the extension of the predicted values of the state and error covariance terms in the Kalman Filter.

The monitor management scheme proposed in Chapter 5 requires the extension of the predicted value of the state estimate error covariance matrix over times when no measurements are taken. This requires modifications to the basic Kalman Filter algorithm of Chapter 4. Consider the filter equations rewritten as

$$\underset{\sim}{P}_{K+1}^{K} = \underset{\sim}{\Phi}_{K+1}^{K}\underset{\sim}{P}_{K}^{K}\underset{\sim}{\Phi}_{K+1}^{K\,T} + \underset{\sim}{\Omega}_{K+1} \tag{4.27}$$

$$\underset{\sim}{P}_{K}^{K} = \left[\underset{\sim}{I} - \underset{\sim}{G}_{K}\underset{\sim}{C}_{K}\right]\underset{\sim}{P}_{K}^{K-1} \tag{C.1}$$

$$\underset{\sim}{G}_{K} = \underset{\sim}{P}_{K}^{K-1}\underset{\sim}{C}_{K}^{T}\left[\underset{\sim}{C}_{K}\underset{\sim}{P}_{K}^{K-1}\underset{\sim}{C}_{K}^{T} + \underset{\sim}{V}_{K}\right]^{-1} \tag{C.2}$$

For the case of prediction only, no measurements are taken, so set $\underset{\sim}{C}_{K} \equiv 0$ and (see Bryson and Ho [26], p. 361), let

$$\underset{\sim}{V}_{K} \longrightarrow \infty\underset{\sim}{I}$$

$$\Longrightarrow \underset{\sim}{G}_{K} \longrightarrow \underset{\sim}{0} \tag{C.3}$$

$$\Longrightarrow \underset{\sim}{P}_{K}^{K} \longrightarrow \underset{\sim}{P}_{K}^{K-1}$$

so that

$$\underset{\sim}{P}_{K+1}^{K} = \underset{\sim}{\Phi}_{K+1}^{K}\underset{\sim}{P}_{K}^{K-1}\underset{\sim}{\Phi}_{K+1}^{K\,T} + \underset{\sim}{\Omega}_{K+1}. \tag{C.4}$$

Thus, for the case of no measurements, the predicted error covariance matrix may be calculated iteratively as a function of its own past values and the state noise uncertainty term $\underset{\sim}{\Omega}_{K+1}$.

Equation (C.4) serves as the heart of the prediction process for $\underset{\sim}{P}^{K}_{K+N}$, which is the value of the error covariance matrix predicted ahead N steps to time t_{K+N} but based only on the knowledge of measurements made through time t_K. In practice, a fixed time interval $T \equiv (t_{K+1} - t_K)$ is chosen so that

$$\underset{\sim}{\Phi}^{K}_{K+1} = \underset{\sim}{\Phi}\left(t_{K+1}, t_K\right) = \underset{\sim}{\Phi}(T) \equiv \underset{\sim}{\Phi} = e^{\underset{\sim}{A}T} \tag{C.5}$$

$$\underset{\sim}{\Omega}_{K+1} = \underset{\sim}{\Omega}\left(t_{K+1} - t_K\right) = \underset{\sim}{\Omega}(T) \equiv \underset{\sim}{\Omega} \tag{C.6}$$

(see Appendixes A and B for details). With this computational time step T, it is possible to formulate an expression for $\underset{\sim}{P}^{K}_{K+N}$.

First note that for fixed size time steps, $\underset{\sim}{\Omega}$ in (C.6) is a constant, that is,

$$\underset{\sim}{\Omega} \equiv \underset{\sim}{\Omega}_{K+1} \equiv \underset{\sim}{\Omega}_{J+1}, \qquad \text{all K and J.} \tag{C.7}$$

$\underset{\sim}{\Omega}$ represents the <u>per step</u> increase in the uncertainty in the state estimate due to the stochastic input acting upon the state. Thus if the statistics of $\underset{\sim}{w}(t)$ in (4.14) are constant, that is, if

$$\underset{\sim}{W}(t) = \underset{\sim}{W}(\tau), \qquad \text{all t and } \tau \tag{C.8}$$

Then from Appendix B, for fixed step size, $\underset{\sim}{\Omega}$ is a constant. With (C.5) and (C.6), (C.4) becomes

$$\underset{\sim}{P}^{K}_{K+1} = \underset{\sim}{\Phi}\underset{\sim}{P}^{K-1}_{K}\underset{\sim}{\Phi}^{T} + \underset{\sim}{\Omega}. \tag{C.9}$$

The recursion to obtain $\underset{\sim}{P}^{K}_{K+N}$ starts from the corrected error covariance matrix at time t_K, $\underset{\sim}{P}^{K}_{K}$, and predicts ahead one-step,

$$\underset{\sim}{P}^{K}_{K+1} = \underset{\sim}{\Phi}\underset{\sim}{P}^{K}_{K}\underset{\sim}{\Phi}^{T} + \underset{\sim}{\Omega}. \tag{C.10}$$

Subsequent steps are taken using (C.9),

$$\begin{aligned}\underset{\sim}{P}^{K}_{K+2} &= \underset{\sim}{\Phi}\underset{\sim}{P}^{K}_{K+1}\underset{\sim}{\Phi}^{T} + \underset{\sim}{\Omega} \\ &= \underset{\sim}{\Phi}\left[\underset{\sim}{\Phi}\underset{\sim}{P}^{K}_{K}\underset{\sim}{\Phi}^{T} + \underset{\sim}{\Omega}\right]\underset{\sim}{\Phi}^{T} + \underset{\sim}{\Omega} \\ &= \underset{\sim}{\Phi}^{2}\underset{\sim}{P}^{K}_{K}\underset{\sim}{\Phi}^{2T} + \underset{\sim}{\Phi}\underset{\sim}{\Omega}\underset{\sim}{\Phi}^{T} + \underset{\sim}{\Omega}.\end{aligned} \tag{C.11}$$

Finally, for step t_{K+N},

$$\underset{\sim}{P}^{K}_{K+N} = \underset{\sim}{\Phi}^{N}\underset{\sim}{P}^{K}_{K}\underset{\sim}{\Phi}^{N^{T}} + \sum_{n=1}^{N}\underset{\sim}{\Phi}^{n-1}\underset{\sim}{\Omega}\underset{\sim}{\Phi}^{n-1^{T}}. \tag{C.12}$$

The two terms in (C.12) represent the free and driven response of $\underset{\sim}{P}$ as time grows. If $\underset{\sim}{A}$ is stable, the first term decreases with time. The second term, a discrete-time convolution of the forcing term $\underset{\sim}{\Omega}$, grows with time to some steady-state value.

In practice, the prediction is started with (C.10) and then extended recursively using (C.9) until some error limits are reached; say this occurs at time t_{K+N}. Now it is required to extend the state estimate itself to time t_{K+N}. For a fixed time step, from Appendix A,

$$\underset{\sim}{\Psi}^{K}_{K+1} = \underset{\sim}{\Psi}\left(t_{K+1} - t_{K}\right) = \underset{\sim}{\Psi}(T) \equiv \underset{\sim}{\Psi} \tag{C.13}$$

and the predicted and corrected values of the state estimate can be written

$$\hat{\underset{\sim}{x}}^{K}_{K+1} = \underset{\sim}{\Phi}\hat{\underset{\sim}{x}}^{K}_{K} + \underset{\sim}{\Psi}\underset{\sim}{u}_{K} \tag{C.14}$$

$$\hat{\underset{\sim}{x}}^{K}_{K} = \hat{\underset{\sim}{x}}^{K-1}_{K} + \underset{\sim}{G}_{K}\left[\underset{\sim}{y}_{K} - \underset{\sim}{C}_{K}\hat{\underset{\sim}{x}}^{K-1}_{K}\right]. \tag{C.15}$$

From (C.3), the fact that no measurements are taken results in

$$\hat{\underset{\sim}{x}}_K^K \longrightarrow \hat{\underset{\sim}{x}}_K^{K-1} \tag{C.16}$$

$$\hat{\underset{\sim}{x}}_{K+1}^K = \underset{\sim}{\underset{\sim}{\Phi}} \hat{\underset{\sim}{x}}_K^{K-1} + \underset{\sim}{\underset{\sim}{\Psi}} \underset{\sim}{u}_K. \tag{C.17}$$

Thus, the current predicted value of the state estimate may be expressed as a function of its own past values and the past deterministic inputs.

In a manner similar to (C.11), the value of the state estimate predicted ahead N time steps is found to be

$$\hat{\underset{\sim}{x}}_{K+N}^K = \underset{\sim}{\Phi}^N \hat{\underset{\sim}{x}}_K^K + \sum_{n=K}^{\overbrace{K+N-1}} \underset{\sim}{\Phi}^{K+N-1-n} \underset{\sim}{\underset{\sim}{\Psi}} \underset{\sim}{u}_n. \tag{C.18}$$

Thus, once the covariance matrix has been recursively extended ahead to time t_{K+N}, the state estimate may be predicted ahead all at once with (C.18).

APPENDIX D. ANALYTICAL MEASUREMENT OPTIMIZATION

The purpose of this appendix is to demonstrate the difficulties in attempting to solve the measurement placement optimization problem analytically. The problem involves finding the optimum measurement matrix $\underset{\sim}{C}^*$ at a measurement time, time t_{K+N}, which minimizes some performance criterion. Two criteria are considered; one in which the error in the state estimate after the measurement is to be minimized, the other where the sum of estimate error and measurement cost are to be minimized. Both attempts are found to fail.

D.1 Minimize Estimate Error

For the case, the performance criterion is chosen to be

$$J_1 \equiv \mathrm{Tr}\left[\underset{\sim}{P}^{K+N}_{K+N}\right] = \mathrm{Tr}\left[\underset{\sim}{P}^{K}_{K+N} - \underset{\sim}{P}^{K}_{K+N}\underset{\sim}{C}^T\left(\underset{\sim}{C}\underset{\sim}{P}^{K}_{K+N}\underset{\sim}{C}^T + \underset{\sim}{V}\right)^{-1}\underset{\sim}{C}\underset{\sim}{P}^{K}_{K+N}\right]. \tag{D.1}$$

Define

$$\underset{\sim}{T} \equiv \left(\underset{\sim}{C}\underset{\sim}{P}^{K}_{K+N}\underset{\sim}{C}^T + \underset{\sim}{V}\right) \tag{D.2}$$

and drop subscripts for now. Then, following Athans [11], take the total differential of J_1

$$\begin{aligned} dJ_1 &= d\mathrm{Tr}\left[\underset{\sim}{P} - \underset{\sim}{P}\underset{\sim}{C}^T\underset{\sim}{T}^{-1}\underset{\sim}{C}\underset{\sim}{P}\right] \\ &= \mathrm{Tr}\left[\cancel{d\underset{\sim}{P}} - d\left(\underset{\sim}{P}\underset{\sim}{C}^T\underset{\sim}{T}^{-1}\underset{\sim}{C}\underset{\sim}{P}\right)\right] \\ &= \mathrm{Tr}\left[\underset{\sim}{P}\left(d\underset{\sim}{C}^T\right)\underset{\sim}{T}^{-1}\underset{\sim}{C}\underset{\sim}{P} - \underset{\sim}{P}\underset{\sim}{C}^T\underset{\sim}{T}^{-1}\left\{(d\underset{\sim}{C})\underset{\sim}{P}\underset{\sim}{C}^T\right.\right. \\ &\qquad \left.\left. + \underset{\sim}{C}\underset{\sim}{P}\left(d\underset{\sim}{C}^T\right)\right\}\underset{\sim}{T}^{-1}\underset{\sim}{C}\underset{\sim}{P} + \underset{\sim}{P}\underset{\sim}{C}^T\underset{\sim}{T}^{-1}(d\underset{\sim}{C})\underset{\sim}{P}\right]. \end{aligned} \tag{D.3}$$

In (D.3), use was made of the chain rule. The second term may be derived as follows:

To find

$$d\left[\underset{\sim}{C}\underset{\sim}{P}\underset{\sim}{C}^T + \underset{\sim}{Y}\right]^{-1}$$

first let

$$\underset{\sim}{X}\underset{\sim}{Y} = \underset{\sim}{I},$$

$$\underset{\sim}{X} = \underset{\sim}{Y}^{-1}$$

$$\Longrightarrow \quad d(\underset{\sim}{X}\underset{\sim}{Y}) = (d\underset{\sim}{X})\underset{\sim}{Y} + \underset{\sim}{X}(d\underset{\sim}{Y}) = d\underset{\sim}{I} = \underset{\sim}{0}.$$

$$\Longrightarrow \quad d\underset{\sim}{X} = -\underset{\sim}{X}(d\underset{\sim}{Y})\underset{\sim}{Y}^{-1}$$

$$= \underset{\sim}{Y}^{-1}(d\underset{\sim}{Y})\underset{\sim}{Y}^{-1}$$

or

$$d\underset{\sim}{Y}^{-1} = -\underset{\sim}{Y}^{-1}(d\underset{\sim}{Y})\underset{\sim}{Y}^{-1}.$$

Now, if

$$\underset{\sim}{Y} \equiv \left[\underset{\sim}{C}\underset{\sim}{P}\underset{\sim}{C}^T + \underset{\sim}{Y}\right],$$

then

$$d\underset{\sim}{Y} = (d\underset{\sim}{C})\underset{\sim}{P}\underset{\sim}{C}^T + \underset{\sim}{C}\underset{\sim}{P}\left(d\underset{\sim}{C}^T\right)$$

and finally,

$$d\underset{\sim}{Y}^{-1} = -\underset{\sim}{Y}^{-1}\left[(d\underset{\sim}{C})\underset{\sim}{P}\underset{\sim}{C}^T + \underset{\sim}{C}\underset{\sim}{P}\left(d\underset{\sim}{C}^T\right)\right]\underset{\sim}{Y}^{-1}$$

as sought.

Return to (D.3) and expand the second term to obtain

$$dJ_1 = -\mathrm{Tr}\left[\underset{\sim}{P}\left(d\underset{\sim}{C}^T\right)\underset{\sim}{T}^{-1}\underset{\sim}{C}\underset{\sim}{P} - \underset{\sim}{P}\underset{\sim}{C}^T\underset{\sim}{T}^{-1}(d\underset{\sim}{C})\underset{\sim}{P}\underset{\sim}{C}^T\underset{\sim}{T}^{-1}\underset{\sim}{C}\underset{\sim}{P}\right.$$

$$\left. - \underset{\sim}{P}\underset{\sim}{C}^T\underset{\sim}{T}^{-1}\underset{\sim}{C}\underset{\sim}{P}\left(d\underset{\sim}{C}^T\right)\underset{\sim}{T}^{-1}\underset{\sim}{C}\underset{\sim}{P} + \underset{\sim}{P}\underset{\sim}{C}^T\underset{\sim}{T}^{-1}(d\underset{\sim}{C})\underset{\sim}{P}\right]. \qquad (D.4)$$

Bringing the total differential operator d(.) inside the trace operator Tr[.] is valid since both are linear operators, so is the partial differ-

ential operator $\frac{\partial}{\partial x}(\cdot)$. Thus, in order to take the partial derivative of J_1 with respect to the matrix $\underline{C}$, follow Athans ([11], p. 19) with the use of unit matrices $\underline{E}_{ij}$ to obtain

$$\frac{\partial}{\partial \underline{C}} J_1 = \frac{\partial}{\partial \underline{C}} \mathrm{Tr}\left[P^{K+N}_{K+N}\right]$$

$$= -\sum_{ijk} \underline{E}_{ik}\Big[\underline{P}(\underline{E}_{ji})\underline{T}^{-1}\underline{C}\underline{P} - \underline{P}\underline{C}\underline{T}^{-1}(\underline{E}_{ij})\underline{P}\underline{C}^T\underline{T}^{-1}\underline{C}\underline{P}$$

$$- \underline{P}\underline{C}^T\underline{T}^{-1}\underline{C}\underline{P}(\underline{E}_{ji})\underline{T}^{-1}\underline{C}\underline{P} + \underline{P}\underline{C}^T\underline{T}^{-1}(\underline{E}_{ij})\underline{P}\Big]\underline{E}_{kj}$$

$$= \sum_{ijk} -\underline{E}_{ik}\underline{P}\underline{E}_{ji}\underline{T}^{-1}\underline{C}\underline{P}\underline{E}_{kj} + \underline{E}_{ik}\underline{P}\underline{C}\underline{T}^{-1}\underline{E}_{ij}\underline{P}\underline{C}^T\underline{T}^{-1}\underline{C}\underline{P}\underline{E}_{kj}$$

$$+ \underline{E}_{ik}\underline{P}\underline{C}^T\underline{T}^{-1}\underline{C}\underline{P}\underline{E}_{ji}\underline{T}^{-1}\underline{C}\underline{P}\underline{E}_{kj} - \underline{E}_{ik}\underline{P}\underline{C}^T\underline{T}^{-1}\underline{E}_{ij}\underline{P}_{kj}$$

$$= \sum_{ijk} -[\underline{P}]_{kj}\underline{E}_{ii}\underline{T}^{-1}\underline{C}\underline{P}\underline{E}_{kj} + \left[\underline{P}\underline{C}\underline{T}^{-1}\right]_{ki}\underline{E}_{ij}\underline{P}\underline{C}^T\underline{T}^{-1}\underline{C}\underline{P}\underline{E}_{kj}$$

$$+ \left[\underline{P}\underline{C}^T\underline{T}^{-1}\underline{C}\underline{P}\right]_{kj}\underline{E}_{ii}\underline{T}^{-1}\underline{C}\underline{P}\underline{E}_{kj} - \left[\underline{P}\underline{C}^T\underline{T}^{-1}\right]_{ki}\underline{E}_{ij}\underline{P}\underline{E}_{kj}$$

(see [11], Eq. 5-14)

$$= \sum_{ijk} -[\underline{P}]_{kj}\left[\underline{T}^{-1}\underline{C}\underline{P}\right]_{ik}\underline{E}_{ij} + \left[\underline{P}\underline{C}\underline{T}^{-1}\right]_{ki}\left[\underline{P}\underline{C}^T\underline{T}^{-1}\underline{C}\underline{P}\right]_{jk}\underline{E}_{ij}$$

$$+ \left[\underline{P}\underline{C}^T\underline{T}^{-1}\underline{C}\underline{P}\right]_{kj}\left[\underline{T}^{-1}\underline{C}\underline{P}\right]_{ik}\underline{E}_{ij} - \left[\underline{P}\underline{C}^T\underline{T}^{-1}\right]_{ki}[\underline{P}]_{jk}\underline{E}_{ij}$$

(now, with rules of matrix multiplication)

$$= -\underline{T}^{-1}\underline{C}\underline{P}\underline{P} + \underline{T}^{-1^T}\underline{C}^T\underline{P}^T\underline{P}^T\underline{C}^T\underline{T}^{-1^T}\underline{C}\underline{P}^T$$

$$+ \underline{T}^{-1}\underline{C}\underline{P}\underline{P}\underline{C}^T\underline{T}^{-1}\underline{C}\underline{P} - \underline{T}^{-1}\underline{C}\underline{P}^T\underline{P}^T. \qquad \text{(D.5)}$$

Noting that

$$\underset{\sim}{P} = \underset{\sim}{P}^T$$

$$\tilde{\underset{\sim}{T}} = \tilde{\underset{\sim}{T}}^T \qquad \Rightarrow \underset{\sim}{T}^{-1} = \underset{\sim}{T}^{-1^T}$$

(D.5) becomes

$$\frac{\partial}{\partial \underset{\sim}{C}} J_1 = -2\left[\underset{\sim}{T}^{-1}\underset{\sim}{C}\underset{\sim}{P}^2 - \underset{\sim}{T}^{-1}\underset{\sim}{C}\underset{\sim}{P}^2\underset{\sim}{C}\underset{\sim}{T}^{-1}\underset{\sim}{C}\underset{\sim}{P}\right]. \tag{D.6}$$

(D.6) is the relationship sought, the derivation of which may seem obscure. A more simple derivation results from making a pair of identities and the statement of a Lemma [11]:

$$\begin{aligned} &\frac{\partial}{\partial \underset{\sim}{X}} \mathrm{Tr}[\underset{\sim}{A}\underset{\sim}{X}\underset{\sim}{B}] = \underset{\sim}{A}^T\underset{\sim}{B}^T, \\ &\frac{\partial}{\partial \underset{\sim}{X}} \mathrm{Tr}[\underset{\sim}{A}\underset{\sim}{X}^T\underset{\sim}{B}] = \underset{\sim}{B}\underset{\sim}{A}. \end{aligned} \tag{D.7}$$

These follow from

Lemma: If

$$\frac{\partial}{\partial x_{ij}} \mathrm{Tr}[\underset{\sim}{A}\underset{\sim}{X}] = \mathrm{Tr}\left[\underset{\sim}{A}\underset{\sim}{E}_{ij}\right], \qquad \text{then} \qquad \frac{\partial}{\partial \underset{\sim}{X}} \mathrm{Tr}\,[\underset{\sim}{A}\underset{\sim}{X}] = \underset{\sim}{A}^T.$$

To demonstrate the above formulas,

$$d\mathrm{Tr}[\underset{\sim}{A}\underset{\sim}{X}\underset{\sim}{B}] = \mathrm{Tr}\left[\underset{\sim}{A}(d\underset{\sim}{X})\underset{\sim}{B}\right] = \mathrm{Tr}\left[\underset{\sim}{B}\underset{\sim}{A}(d\underset{\sim}{X})\right].$$

Now apply the Lemma:

$$\frac{\partial}{\partial x_{ij}} \mathrm{Tr}[\underset{\sim}{A}\underset{\sim}{X}\underset{\sim}{B}] = \mathrm{Tr}\left[\underset{\sim}{B}\underset{\sim}{A}\frac{\partial}{\partial x_{ij}}\right] = \mathrm{Tr}\left[\underset{\sim}{B}\underset{\sim}{A}\underset{\sim}{E}_{ij}\right] \qquad \frac{\partial}{\partial \underset{\sim}{X}} [\underset{\sim}{A}\underset{\sim}{X}\underset{\sim}{B}] = \underset{\sim}{A}^T\underset{\sim}{B}^T.$$

Similarly,

$$\frac{\partial}{\partial x_{ij}} \mathrm{Tr}\left[\underset{\sim}{A}\underset{\sim}{X}^T\underset{\sim}{B}\right] = \mathrm{Tr}\left[\underset{\sim}{B}\underset{\sim}{A}\underset{\sim}{E}_{ji}\right] \Rightarrow \frac{\partial}{\partial \underset{\sim}{X}} \mathrm{Tr}\left[\underset{\sim}{A}\underset{\sim}{X}^T\underset{\sim}{B}\right] = \underset{\sim}{B}\underset{\sim}{A}.$$

With the use of (D.7), (D.6) can be obtained directly from (D.4) as follows:

$$dJ_1 = -\mathrm{Tr}\Big[\underset{\sim}{P}(d\underset{\sim}{C}^T)\underset{\sim}{T}^{-1}\underset{\sim}{C}\underset{\sim}{P} - \underset{\sim}{P}\underset{\sim}{C}^T\underset{\sim}{T}^{-1}(d\underset{\sim}{C})\underset{\sim}{P}\underset{\sim}{C}^T\underset{\sim}{T}^{-1}\underset{\sim}{C}\underset{\sim}{P} - \underset{\sim}{P}\underset{\sim}{C}^T\underset{\sim}{T}^{-1}\underset{\sim}{C}\underset{\sim}{P}(d\underset{\sim}{C}^T)\underset{\sim}{T}^{-1}\underset{\sim}{C}\underset{\sim}{P} + \underset{\sim}{P}\underset{\sim}{C}^T\underset{\sim}{T}^{-1}(d\underset{\sim}{C})\underset{\sim}{P}\Big]. \tag{D.4}$$

$$\Rightarrow \frac{\partial}{\partial \underset{\sim}{C}} J_1 = -\underset{\sim}{T}^{-1}\underset{\sim}{C}\underset{\sim}{P}\underset{\sim}{P} + \underset{\sim}{T}^{-1}\underset{\sim}{C}\underset{\sim}{P}\underset{\sim}{P}^T\underset{\sim}{C}^T\underset{\sim}{T}^{-1}{}^T\underset{\sim}{C}\underset{\sim}{P}^T + \underset{\sim}{T}^{-1}\underset{\sim}{C}\underset{\sim}{P}\underset{\sim}{P}\underset{\sim}{C}^T\underset{\sim}{T}^{-1}\underset{\sim}{C}\underset{\sim}{P} - \underset{\sim}{T}^{-1}\underset{\sim}{C}\underset{\sim}{P}^T\underset{\sim}{P}^T$$

$$= -2\Big[\underset{\sim}{T}^{-1}\underset{\sim}{C}\underset{\sim}{P}^2 - \underset{\sim}{T}^{-1}\underset{\sim}{C}\underset{\sim}{P}^2\underset{\sim}{C}^T\underset{\sim}{T}^{-1}\underset{\sim}{C}\underset{\sim}{P}\Big] \tag{D.6}$$

as before.

Now, in the measurement optimization problem, we seek an extremal in $\underset{\sim}{C}$, $\underset{\sim}{C}^*$, which minimizes $J_1 \equiv \mathrm{Tr}\left[P^{K+N}_{K+N}\right]$. To that end, set

$$\frac{\partial}{\partial \underset{\sim}{C}} J_1 = \underset{\sim}{0}. \tag{D.8}$$

$$\underset{\sim}{T}^{-1}\underset{\sim}{C}\underset{\sim}{P}\Big[\underset{\sim}{P} - \underset{\sim}{P}\underset{\sim}{C}^T\Big(\underset{\sim}{C}\underset{\sim}{P}\underset{\sim}{C}^T + \underset{\sim}{V}\Big)^{-1}\underset{\sim}{C}\underset{\sim}{P}\Big] = \underset{\sim}{0}. \tag{D.9}$$

Simplify (D.9) with the use of

Lemma: Matrix Inversion (see [78])

For $\underset{\sim}{P} > 0$, $\underset{\sim}{V} > 0$

$$\underset{\sim}{P} - \underset{\sim}{P}\underset{\sim}{C}^T\Big(\underset{\sim}{C}\underset{\sim}{P}\underset{\sim}{C}^T + \underset{\sim}{V}\Big)^{-1}\underset{\sim}{C}\underset{\sim}{P} = \Big(\underset{\sim}{P}^{-1} + \underset{\sim}{C}^T\underset{\sim}{V}^{-1}\underset{\sim}{C}\Big)^{-1}. \tag{D.10}$$

To prove that this is true, simply multiply both sides by the inverse of the right-hand side and collect terms. Substituting (D.10) into (D.9), obtain

$$\frac{\partial}{\partial \underset{\sim}{C}} J_1 = \underset{\sim}{T}^{-1}\underset{\sim}{C}\underset{\sim}{P}\Big[\underset{\sim}{P}^{-1} + \underset{\sim}{C}^T\underset{\sim}{V}^{-1}\underset{\sim}{C}\Big]^{-1}$$

$$= \cancel{\underset{\sim}{T}^{-1}\underset{\sim}{C}\underset{\sim}{P}}$$

$$= \underset{\sim}{C} = \underset{\sim}{0}. \tag{D.11}$$

Thus, the extremalization results in the value $\underset{\sim}{C}^* = \underset{\sim}{0}$. However, this is only a necessary condition, and obviously corresponds to a maximum in the performance criterion. Noting the form of J_1 in (D.1), the negative sign in front of the second term shows that for any $\hat{\underset{\sim}{C}} \neq \underset{\sim}{0}$, $\hat{J}_1 < J_1^*$, that is, the extremal found is a maximum. This corresponds to the case where no measurements are taken. The value of J_1 from (D.1) for $\underset{\sim}{C}^* = \underset{\sim}{0}$ can be seen to be equal to $\mathrm{Tr}\left[\underset{\sim}{P}_{K+N}^{K+N}\right] = \mathrm{Tr}\left[\underset{\sim}{P}_{K+N}^{K}\right]$, that is, the predicted and corrected covariance matrices are equal, which agrees with the case when no measurements are taken.

The opposite extreme is of some interest, that is, the case where the "size" of the matrix $\underset{\sim}{C}$, as given by its norm, grows without bound, $\left\|\underset{\sim}{C}\right\| \to \infty$. Consider the case where $\underset{\sim}{C}$ is square and nonsingular. Then, from (D.1), dropping subscripts we find as $\left\|\underset{\sim}{C}\right\| \to \infty$,

$$\begin{aligned}
\mathrm{Tr}\left[\underset{\sim}{P}_{K+N}^{K+N}\right] &= \mathrm{Tr}\left[\underset{\sim}{P} - \underset{\sim}{P}\underset{\sim}{C}^T\left(\underset{\sim}{C}\underset{\sim}{P}\underset{\sim}{C}^T + \underset{\sim}{V}\right)^{-1}\underset{\sim}{C}\underset{\sim}{P}\right] \\
&\to \mathrm{Tr}\left[\underset{\sim}{P} - \underset{\sim}{P}\underset{\sim}{C}^T\left(\underset{\sim}{C}\underset{\sim}{P}\underset{\sim}{C}^T\right)^{-1}\underset{\sim}{C}\underset{\sim}{P}\right] \\
&= \mathrm{Tr}\left[\underset{\sim}{P} - \underset{\sim}{P}\underset{\sim}{C}^T\left(\underset{\sim}{C}^{T-1}\underset{\sim}{P}^{-1}\underset{\sim}{C}^{-1}\right)\underset{\sim}{C}\underset{\sim}{P}\right] \\
&= \mathrm{Tr}[\underset{\sim}{P} - \underset{\sim}{P}] = \underset{\sim}{0}.
\end{aligned} \tag{D.12}$$

This is the result we would expect. As can be seen from Eq. (4.17) for the filter,

$$\underset{\sim}{y}_{K+N} = \underset{\sim}{C}_{K+N}\underset{\sim}{x}_{K+N} + \underset{\sim}{v}_{K+N}, \tag{D.13}$$

the "larger" $\underset{\sim}{C}_{K+N}$, the more deterministic information is contained in $\underset{\sim}{y}_{K+N}$ and the greater the signal-to-noise ratio. This manifests itself in the variances of the estimates of the states going to zero, as seen in the diagonal terms of $\underset{\sim}{P}_{K+N}^{K+N}$ vanishing. The quadratic term dominates the measurement noise covariance $\underset{\sim}{V}$ in the expression to be inverted which allows our limiting operation to take place.

It should be noted here that even if this analysis had led to useful results, a major constraint is placed upon the result in that the operations of taking derivatives of traces of matrices (as in (D.5) and (D.7)) are based upon the utilization of unit matrices E_{ij} which are square matrices. Thus, only in the case where C is a square matrix, i.e., as many measurement devices as states, could this analysis apply. This is a serious limitation in the context of studying the optimization of measurement systems.

D.2 Minimize Estimation Error and Measurement Cost

To alleviate the degeneracy found above, let

$$J_2 \equiv \mathrm{Tr}\left[P^{K+N}_{K+N} + C^T_{K+N} Q C_{K+N}\right]$$

$$= \mathrm{Tr}\left[P^K_{K+N} - P^K_{K+N} C^T_{K+N}\left(C_{K+N} P^K_{K+N} + V\right)^{-1} C_{K+N} P^K_{K+N} + C^T_{K+N} Q C_{K+N}\right] \quad (D.14)$$

Let $T \equiv (CPC^T + V)$.

Then

$$dJ_2 = d\mathrm{Tr}\left[P + C^T Q C\right]$$

$$= \mathrm{Tr}\Big[-P\left(dC^T\right)T^{-1}CP$$

$$+ PC^T T^{-1}\left\{(dC)PC^T + CP\left(dC^T\right)\right\}T^{-1}CP$$

$$- PC^T T^{-1}(dC)P + \left(dC^T\right)QC + C^T Q(dC)\Big]$$

$$= \mathrm{Tr}\Big[- P\left(dC^T\right)T^{-1}CP + PC^T T^{-1}(dC)PC^T T^{-1}CP$$

$$+ PC^T T^{-1}CP\left(dC^T\right)T^{-1}CP$$

$$- PC^T T^{-1}(dC)P + \left(dC^T\right)QC + C^T Q(dC)\Big]. \quad (D.15)$$

And

$$\frac{\partial}{\partial C} J_2 = -T^{-1}CPP + T^{-1^T}CP^TP^TC^TT^{-1^T}CP^T$$

$$+ T^{-1}CPPC^TT^{-1}CP - T^{-1^T}CP^TP^T + QC + Q^TC - Q$$

$$= -2\left\{T^{-1}CP^2 - T^{-1}CP^2C^TT^{-1}CP - QC\right\} = Q$$

$$= T^{-1}CP\left[P - PC^T\left(CPC^T\right) + V^{-1}CP\right] - QC$$

$$= T^{-1}CP\left(P^{-1} + C^TV^{-1}C\right)^{-1} - QC$$

$$= CP - \left(CPC^T + V\right)QC\left(P^{-1} + C^TV^{-1}C\right) = Q$$

$$= CPC^TQCP^{-1}\ P\ CPC^TQCC^TV^{-1}C$$

$$+ VQCP^{-1} + VQCC^TV^{-1}C - CP = Q. \qquad (D.16)$$

Thus, extremalization with respect to a combined performance index, one which includes a weighted term for measurement cost, results in a very complicated expression.

Now, operate on the above equation to obtain

$$CPC^TQCP^{-1} + CPC^TQCC^TV^{-1}C + VQCP^{-1} + VQCC^TV^{-1}C - CP = Q. \quad (D.17)$$

Assume C^{-1} exists. Thus,

$$PC^TQC + PC^TQCC^TV^{-1}CP + C^{-1}VQC + C^{-1}VQCC^TV^{-1}CP - P^2 = Q. \quad (D.18)$$

or, finally,

$$P\left(C^TQC\right) + \left(C^{-1}VQCC^TV^{-1}C\right)P + C^{-1}VQC$$

$$- P\left(I - C^TQCC^TV^{-1}C\right)P = Q. \qquad (D.19)$$

Discussion: The drawback of the above equation is that it solves for the wrong variable, $\underset{\sim}{P}^{K}_{K+N}$, in terms of $\underset{\sim}{C}_{K+N}$; required is the opposite, to solve for $\underset{\sim}{C}_{K+N}$ as a function of $\underset{\sim}{P}^{K}_{K+N}$ which is known at time K+N.

The equation could be used iteratively to find the $\underset{\sim}{P}$ which matches the $\underset{\sim}{P}^{K}_{K+N}$ already known in order to find the $\underset{\sim}{C}_{K+N}$; this type of method is not desirable, however.

Also, to get $\frac{\partial}{\partial \underset{\sim}{C}} J_2$ into the form of a Riccati equation as in (D.19), for which standard solutions exist, a necessary assumption was that $\underset{\sim}{C}_{K+N}$ be nonsingular. This implies having as many measurements as states at each measurement time which is a severe limitation when the point of the problem included minimizing the necessary number of measurements.

D.3 Results

Choices of the two performance criteria J_1 and J_2, show that obtaining an extremum analytically is very elusive. No modification made by this author to the above performance criteria led to a set of equations for which an analytical solution could be found.

More importantly, the fundamental concept of minimizing some performance criterion with respect to the whole measurement matrix $\underset{\sim}{C}$ itself seems like the wrong thing to do. By this is meant that the elements of $\underset{\sim}{C}$ in a general formulation of the system equations have little to do with the placement of measurement sites. An exception to this would be the case of decoupled state measurement where the model could be discretized in space with one sensor in each element of the finite difference representation.

Another possibility would be the formulation of the system in normal mode coordinates. In this case, the $\underset{\sim}{C}$ matrix has a very definite

structure, where the sensor placements $\underset{\sim}{z}$ appear as arguments of the matrix $\underset{\sim}{C} = \underset{\sim}{C}(\underset{\sim}{z})$.

The former case, with a diagonal matrix $\underset{\sim}{C}$, was difficult to get into a form where optimal measurement locations would result. In the latter case, that of normal modes, a way was not found to constrain the solution to fit the normal mode form for $\underset{\sim}{C}$.

Also, the addition of the quadratic term in $\underset{\sim}{C}$ in J_2 above is difficult to understand. It was meant to represent measurement cost but in problem structure here, any direct connection with cost of measurement is unclear.

For these reasons, a more fundamental approach was decided upon, that of minimizing the performance index directly with respect to the vector of sensor positions $\underset{\sim}{z}$. The problem is also to be formulated in normal modes, in order to simplify computation and also to direct the measurement positions to the problem structure through the measurement matrix $\underset{\sim}{C}(\underset{\sim}{z})$. The minimization is done for various dimensions of $\underset{\sim}{z}$, representing various numbers of sensors. Thus, measurement cost is directly related to the dimension of $\underset{\sim}{z}$.

APPENDIX E. NUMERICAL MEASUREMENT QUALITY OPTIMIZATION

As mentioned in Section 5.3.7, the inclusion of the optimal selection o the *types* of measurement sensors to deploy at a measurement time depends upon the way in which the measurement cost is defined in the original optimal monitoring problem definition.

The case outlined in this Appendix deals with measurement cost which is defined to be proportional to measurement instrument quality; this is the general case first proposed in the optimal monitoring problem statement in Section 2.2. This is a realistic case in which a *discrete* valued measurement cost function could be seen to apply as a function of the specific choices of measurement instrument accuracy which could be obtained commercially. In order to include the quality of measurement devices in the optimal design structure at each measurement time, formulate the portion of the objective function associated with measurement instrument quality first as a *continuous* function of the sizes of the measurement errors, or variances, given by the diagonal elements of the measurement noise covariance matrix $\underset{\sim}{V}$, that is, the terms $[\underset{\sim}{V}]_{ii}$, $i = 1,2,\ldots,m$. The optimal choice of measurement instrument accuracies would then be related to the resulting optimal values for the variances $[\underset{\sim}{V}^*]_{ii}$; the best instrument accuracies would then be those commercially available discrete choices which most closely correspond to the optimal measurement errors of values $[\underset{\sim}{V}^*]_{ii}$, $i = 1,2,\ldots,m$.

To obtain the longest times between required measurements, it seems plausible then to form an adjoined vector for the optimization in Section 5.3.6, a vector composed of the measurement sensor position, z^K *and* their variances *diag* $[\underset{\sim}{V}]$, as follows:

$$\zeta_K \equiv \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_m \\ v_{11} \\ v_{22} \\ \vdots \\ v_{mm} \end{bmatrix}; \quad z_i \equiv \left\{z_K\right\}_i, \quad v_{ii} \equiv [V]_{ii}. \tag{E.1}$$

To include selection of sensor accuracy in the optimization, simply substitute the $2m$-vector ζ_K in (E.1) for m-vector z_K in the definition (5.44) to obtain $J(\zeta_K)$, the combined objective function for measurement position and quality optimization.

A corresponding minor modification to the gradient in (5.49), with T defined as in (5.48), results in the following:

$$\begin{aligned} \frac{\partial}{\partial \zeta_K} J(\zeta_K) = \sum_{i=1}^{m} \Bigg\{ & - e_i \Bigg[P_K^0 \left(\frac{\partial}{\partial z_i} G(\zeta_K) \right)^T T^{-1} G(\zeta_K) P_K^0 \\ & - P_K^0 G(\zeta_K)^T T^{-1} \left\{ \left(\frac{\partial}{\partial z_i} G(\zeta_K) \right) P_K^0 G(\zeta_K)^T + G(\zeta_K) P_K^0 \left(\frac{\partial}{\partial z_i} G(\zeta_K) \right)^T \right\} T^{-1} G(\zeta_K) P_K^0 \\ & + P_K^0 G(\zeta_K)^T T^{-1} \left(\frac{\partial}{\partial z_i} G(\zeta_K) \right) P_K^0 \Bigg]_{11} \\ & + e_{m+1} \left[P_K^0 G(\zeta_K)^T T^{-1} \left\{ E_{ii} \right\} T^{-1} G(\zeta_K) P_K^0 \right]_{11} \Bigg\}, \end{aligned} \tag{E.2}$$

where, from the definition of ζ_K in (E.1),

$$\frac{\partial}{\partial \zeta_{m+i}} V \equiv \frac{\partial}{\partial V_{ii}} V = E_{ii} \tag{E.3}$$

(see Athans and Schweppe [11], Equation (7.17)). Thus, the combined gradient in (E.2) can be simply seen to be

$$\frac{\partial}{\partial \underset{\sim}{\zeta}_K} J(\underset{\sim}{\zeta}_K) = \begin{bmatrix} \frac{\partial}{\partial \underset{\sim}{\zeta}_K} J(\underset{\sim}{\zeta}_K) \\ - - - - - - - - \\ \frac{\partial}{\partial diag\ [\underset{\sim}{V}]} J(\underset{\sim}{V}) \end{bmatrix}, \qquad (E.4)$$

an adjoined $2m$-vector of terms associated with $\underset{\sim}{z}_K$ and $\underset{\sim}{V}$.

Note that finding $\underset{\sim}{\zeta}_K^*$ at the first sample, under the conditions of Conclusion VI, completes the design problem for all other sample times to yield the final result stated as Conclusion VIII in Section 5.3.7.

Notice that the main objective of every optimization problem in the monitoring design problem considered thus far has been to minimize the total *number* of samples taken over all necessary measurement times within the time interval of interest. Adding selection of measurement *instrument quality* to the problem probably changes the design objective to one which seeks to minimize instead the total measurement *cost* as first discussed in Section 2.2 where more accurate measurements (smaller $[\underset{\sim}{V}]_{ii}$) result in higher unit measurement costs. This presents a tradeoff between using numerous low accuracy sensors and fewer high accuracy measurement devices. This restructuring of the problem could easily be carried out with constraints placed upon available measurement instrument accuracies of the form

$$V_{min} \leq [\underset{\sim}{V}]_{ii} \leq V_{max}, \qquad i = 1,2,\ldots,m. \qquad (E.5)$$

These constraints, entered as bounds on the bottom half of $\underset{\sim}{\zeta}_K$ in the gradient minimization algorithm, would lead to optimal values for $\underset{\sim}{\zeta}_K^*$ for the entire range of possible dimensions for $\underset{\sim}{z}_K$, $m = 1,2,\ldots,n$. The optimal results for $\underset{\sim}{\zeta}_K^*$ over all m at the first measurement time, t_K, could then be extended over the whole time interval to determine which choice leads to the lowest total cost; according to Conclusion VII, this

optimal choice for $[\underline{Y}^*]$ at the first sample time must be optimal for all other measurement times, completing the design.

The concepts of this Appendix for the inclusion of measurement instrument quality into the optimal monitoring design problem are presented to indicate how such an extension might be made. The details, though an important part of any realistic design, are not crucial to the other results for the infrequent sampling problem and are omitted in the interest of brevity.

APPENDIX F. DESCRIPTION AND LISTING OF PROGRAM KALMAN

The major computer program written for this study is PROGRAM KALMAN. It contains all the necessary coding for the optimal monitoring design and management computations. It is written in FORTRAN IV for a CDC 7600 computer. It accepts input via a card deck named INFILE and generates an answer file OUTFILE which is given to an ordinary lineprinter. Binary disc files for intermediate storage are generated for use by the graphics package of postprocessor programs listed in Appendix G; these two binary files are called PFILE and TFILE. A flow chart of the interconnections among KALMAN, its input and output files and its postprocessors is shown in Figure F.1. The various computer-generated figures in this report, listed with the programs from which they originated, are included in Figure F.2.

The listing for PROGRAM KALMAN is included in this Appendix. A nearly sufficient number of comment cards are included to permit usage directly. A detailed explanation of its use is omitted here in the interest of brevity; the interested user should examine SUBROUTINE INPUT (lines 402 to 535) where all input statements for the file INFILE occur.

A brief description is now given of the more important routines which comprise this program. KALMAN is the main routine where the Kalman Filter algorithm of Figure 4.1 is implemented, along with the logic associated with solution of the optimal monitoring problems as given in Conclusions II, III, X, and XI. SUBROUTINE FVAL computes $[\underset{\sim}{P}_K^K(\underset{\sim}{z}_K)]_{11}$ used in the optimizations in SUBROUTINE KEELE for the optimal design problem; SUBROUTINE GRADNT is its first-order gradient, that is, $\frac{\partial}{\partial \underset{\sim}{z}_K} [\underset{\sim}{P}_K^K(\underset{\sim}{z}_K)]_{11}$.

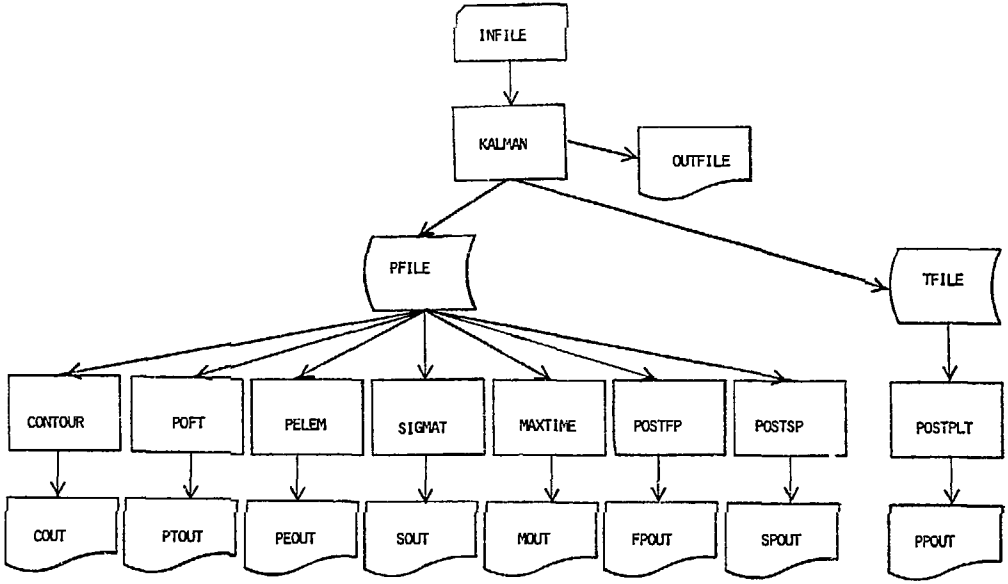


Figure F.1. Relationships among PROGRAM KALMAN, its input and output files and its postprocessors.

PROGRAM	FIGURES GENERATED BY VARIOUS PROGRAMS
KALMAN	6.2, 6.3, 6.4, 6.5, 6.13, 6.17, 6.20, 6.22, 6.24, 6.26, 6.29, 6.31, 6.32
CONTOUR	6.21, 6.23, 6.25, 6.27, 6.28, 6.30, 6.35, 6.40, 6.43, 6.44
POFT	6.6, 6.7, 6.14, 6.15
PELEM	6.8, 6.10
SIGMAT	6.18, 6.19
MAXTIME	6.12
POSTPLT	6.11, 6.33, 6.34, 6.39, 6.41, 6.42, 6.46
POSTFP	6.37
POSTSP	6.38, 6.45

Figure F.2. List of computer-generated figures and the programs from which they came.

SUBROUTINE CONSTR defines the linear inequality constraints of the form (5.53) used in KEELE. TRPKK and DTRPKK define $\mathrm{Tr}[\underset{\sim}{P}_K^K(\underset{\sim}{z}_K)]$ and its gradient, also used in KEELE (they are only used in the comparison of performance criteria found in Section 6.2.3). SUBROUTINE SS computes the check for the approach to steady-state monitoring as in step (3) of (5.72). MAXSIG finds z^*, the position of maximum variance in the output estimate, using SUBROUTINE MUELLER [61] as a root-finder.

SUBROUTINE KEELEA is this author's modification of the original linearly constrained nonlinear programming algorithm KEELE written by G. W. Westley [127]; the addition of a set of random starting vectors has been added to the original routine (see lines 986 through 1000). Subroutines CONDRP, PROJCT, CONADD, CUBMIN, and PRBOLC are all routines from the original KEELE package.

SUBROUTINE PAYNTER finds the number of terms necessary in the matrix series expansion of $\underset{\sim}{\Phi} \equiv e^{\underset{\sim}{A}T}$, the matrix exponential state transition matrix as discussed in Chapter 4 and Appendix A. SUBROUTINE STM performs the actual calculation of $\underset{\sim}{\Phi}_{K+1}^{K}$, $\underset{\sim}{\Psi}_{K+1}^{K}$ and $\underset{\sim}{\Gamma}_{K+1}^{K}$ in (4.12) for the discrete-time state equation. It also performs the computation for $\underset{\sim}{\Omega}_{K+1}$ in (4.14) and (4.15) as suggested by D'Appolito [29] and detailed in Appendix B of this report.

A number of matrix arithmetic algorithms are included (lines 2076 through 2178) whose use was found to greatly simplify the numerous matrix computations which arose in the solutions of the monitoring problems. SUBROUTINE INVERSE (lines 2179 through 2371) is based upon the LDU decomposition reported in Forsythe and Moler [38]; it is recognized as an extremely accurate matrix inversion algorithm.

NOISE, NOISEW, and NOISEV generate normally-distributed random vectors. They use FUNCTION GN which is an implementation of the polar method of generating random deviates from a uniform distribution as reported in Knuth [71]. FUNCTION RAND returns a uniformly-distributed pseudo-random number on the open interval (0,1); it was coded by F. N. Fritsch [42] and is completely portable in that is is useable on any binary computer regardless of its machine word length.

UBAR and UI generate the deterministic forcing function vector $\underset{\sim}{u}(t)$ in (4.1). A selection of possible analytical functions of time are included; see the listing for details.

A number of output routines complete the program, the more notable of which are XYPLOTS and ENDPTS, written by H. K. McCue [84]. These routines provide the line printer plots of $\mathrm{Tr}[\underset{\sim}{P}_{K+N}^{K}]$ and σ_{K+N}^{2} as functions of time t_{K+N} included in this study.

It should be mentioned that extensions of KALMAN to handle more complex problems could be easily accomplished. The eigensystem which results from the boundary conditions of the particular problem under study is specified in SUBROUTINE INPUT; problems other than that of one-dimensional diffusion with scavenging and no-flow boundary conditions as coded in this program can easily be included. By moving the calls to PAYNTER (line 119), STM (123), SS (124), and MAXSIG (127) inside the main integration loop in KALMAN, the loop between statements 20 and 100 (lines 141 and 349), time-varying system matrices and statistics could be included. To handle nonlinearities, the basic Kalman Filter algorithm of Figure 4.1 could be modified to the form of the Extended Kalman Filter with some effort (see Jazwinski [65], Theorem 8.1); the basic structure of this program permits such a direct extension.

Future work should include the development of a more complete inventory of pollutant source models. Besides point sources, representations for distributed background level and line sources in normal model form would broaden the scope of applicability of this program.

```
      PROGRAM KALMAN (INFILE,TAPE2=INFILE,OUTFILE,TAPE3=OUTFILE,
     2                PFILE,TAPE4=PFILE,TFILE,TAPE5=TFILE)
      VER = 10HVER4/30/75
C
      CALL CHANGE (7H1+KALMAN)
      COMMON /10/ NIN,NOUT,NTTY,NRUN,VER
C
      CALL CREATE (5HPFILE,10000,SWT)
      INTEGER POUT
      POUT = 4
      CALL CREATE (5HTFILE,10000,SWT)
      INTEGER TOUT
      TOUT = 5
C
      DIMENSION
C     DIMENSIONS OF FOLLOWING CARDS ARE DEFINED ONLY BY PROBLEM SIZE ND
     1 A(10,10),B(10,10),C(10,10),D(10,10),AC(10,10),BC(10,10),DC(10,10)
     2 ,MO(10),CAPMO(10,10),V(10),CAPV(10,10),W(10),CAPW(10,10),
     3 X(10),XKM1(10),XHKM1K(10),XHKK(10),Y(10),YH(10),Z(10),E(10),
     3 COV(10)
     4 SIGMAV(10),SIGMAW,10),G(10,10),P(10,10),PP(10,10),ID(10,10),
     5 U(10),IU(10),UK(10,3),WI(10,10),W2(10,10),W3(10,10),DY(10),
     6 ZU(10),ZW(10),WKP1(10,10)
C     DIMENSIONS ON FOLLIWNG CARDS ARE DEFINED BY NUMBER OF TIME
C     POINTS TO BE STORED FOR OUTPUT (NT), PROBLEM SIZE (ND), AND
C     NUMBER OF INDIVIDUAL VECTORS OR MATRIX COLUMNS TO BE STORED
C     FOR PLOTTING AND OUTPUT (NP).  DIMENSIONS OF (IOUT) AND (IPLT)
C     COINCIDE WITH NUMBER OF CHOICES FOR OUTPUT AT STATMENT 20 OF
C     MAIN PROGRAM AND NUMBER OF CHOICES FOR DEBUGGING OUTPUT IN DEBUG.
     7 TST(110),ST(110,10,5),JMAX(5),NAMEST(5),NCOLST(5),
     8 IOUT(10),IPLT(5),XYPW1(110),XYPW2(110),TITLES(4,8)
      DIMENSION WSS(10,10),SYMBERR(2)
      DATA SYMBERR / 3HTRP,3HSIG /
      REAL MD,ID
      INTEGER FMAX
      COMMON /PRC3/ N,M,ZMAX,A,P,CAPV,WKP1,WSS,ISING
      EXTERNAL FVAL,GRADNT,CONSTR
      EXTERNAL TRPKK,DTRPKK
      PI = 3.14159265
C     SET SIZE OF ARRAY DIMENSIONS HERE...
      ND = 10
      NT = 110
      NP = 5
C             = THE MAXIMUM PROBLEM SIZE TO BE RUN (LENGTH OF X-VECTOR)
C             = THE MAXIMUM NUMBER OF POINTS TO BE STORED FOR OUTPUT
C               (CAUTION...THIS DIMENSION IS USED IN THE 3-DIMENSIONAL
C               ARRAY (ST(NT,ND,NP)), THUS, IT RAPIDLY ADDS STORAGE
C               TO LENGTH OF PROGRAM.)
C     NP        = THE MAXIMUM NUMBER OF VECTORS TO BE STORED
C     WHERE, NP = (4 * ND), AS PROGRAMMED, IN ORDER TO STORE
C     THE FOLLOWING...(X, XH, E, COV AND ALL M COLUMNS OF G).
C     HERE, M CAN BE AS LARGE AS ND.
C
C     HERE, THE FOLLOWING EQUALITIES ARE MADE FOR THE CALLS TO (OUTPUT3)
      NI = 110
      NJ = ND
      NK = NP
C
C     HERE, IMAX, THE ACTUAL NUMBER OF POINTS TO BE STORED, IS SET
C     EQUAL TO NT, THE DIMENSIONS OF ASSICIATED ARRAYS.  IT COULD BE
C     SET SMALLER IF DESIRED, BUT UNUSED STORAGE WOULD RESULT.
      IMAX = NT
C
C     SET LOGICAL INPUT/OUTPUT UNIT NUMBERS HERE...
      NIN = 2
      NOUT = 3
      NTTY = 59
C     INITIALIZE RUN COUNTER AND START FIRST RUN...
      NRUN = 0
    1 NRUN = NRUN + 1
      CALL INPUT (N,L,M,LL,NTL,IPLT,IOUT,LENGTH,
     2 TO,TI,DT,AC,BC,C,DC,IU,UK,
     3 MO,CAPMO,W,CAPW,V,CAPV,IERROR,NOPQ,EPS,KMAX,TITLES,ND,
     4 Z,ZU,ZW,ZMAX,ERRLIM,LIMIT,ALPHA,NSEARCH,SYMBERR,
     5 NLIN,FMAX,IW,CONVG,DELT,EPSLON,RHO,DELTAP,FLOWER,ACC,IEXP)
C
      IF (IERROR.EQ.-1) GO TO 99
      IF (IERROR.EQ.-2) GO TO 991
C
C     SET UP CONSTANTS FOR KEELE CALLING SEQUENCE
C
      M2 = M * 2
      NE = 0
      NP1 = N + 1
C
C     INITIALIZATION...
      CALL NOISE (MO,CAPMO,X,N,ND)
C     GENERATE NXN IDENTITY MATRIX (ID)
      DO 3 I=1,N
      DO 2 J=1,N
```

```
  2     ID(I,J) = 0.0
  3     ID(I,I) = 1.0
C       INITIALIZE INITIAL CONDITIONS OF SYSTEM MATRICES.  USE -0.0 FOR
C       THOSE WHICH ARE UNDEFINED AT T=TO.
        DO 10 I=1,N
        DO 9 J=1,N
        G(I,J) = -0.0
        P(I,J)  = CAPMO(I,J)
  9     PP(I,J) = CAPMO(I,J)
        XKM1(I) = X(I)
        XHKK(I) = MO(I)
        Y(I) = -0.0
        YH(I) = -0.0
        E(I) = -0.0
        W(I) = -0.0
        V(I) = -0.0
 10     CONTINUE
        T = TO
        K = 0
        NOP = 0

C
C       COMPUTE STATE, CONTROL AND NOISE TRANSITION MARTICES FOR THE
C       DISCRETE PROBLEM (THEY ARE A(K,K-1), B(K,K-1) AND D(K,K-1))
C       GIVEN THEIR EQUIVALENTS FOR THE CONTINUOUS CASE (AC,BC, AND DC).
C       WKP1 REPRESENTS THE DISCRETIZATION OF CONTINUOUS CONVOLUTION OF
C       CAPW(T) FOR T BETWEEN TK AND TK+1, WHERE CAPW(T) IS THE
C       COVARIANCE MATRIX FOR THE MODEL STOCHASTIC INPUT W(T).
C       FORST, DETERMINE NUMBER OF TERMS TO BE USED IN TRUNCATED SERIES KK
        CALL PAYNTER (KK,KMAX,N,DT,EPS,NOUT,AC,ND)
C       IF PAYNTER CRITERION WAS NOT MET, SET NUMBER OF TERMS
C       IN MATRIX EXPANSION OF EXP(A*T) TO MAXIMUM ALLOWED IN INPUT DECK.
        IF(KK.LT.0) KK = KMAX
        CALL STM (N,L,LL,AC,BC,DC,CAPW,A,B,D,WKP1,KK,DT,ND)
        CALL SS  (N,A,WKP1,100.*EPS,NSS,WSS,ND)
C       NOTE THAT WIDTH OF INTERVALS AND MAXIMUM NUMBER OF ITERATIONS
C       IN FINDING POSITION OF MAXIMUN SIGMA IS PROBLEM-SIZE DEPENDENT...
        IF(LIMIT.EQ.2) CALL MAXSIG(SIGMAX,ZSTAR,1./(5*N),CONVG,5*N)

C
        WRITE(POUT)N,M,LL,NTL,TO,TI,LIMIT
        WRITE(TOUT)N,M,LL,NTL,TO,TI,LIMIT,ERRLIM
        WRITE(POUT)((A(I,J),J=1,N),I=1,N)
        WRITE(POUT)((WKP1(I,J),J=1,N),I=1,N)
        WRITE(POUT)((WSS(I,J),J=1,N),I=1,N)
        WRITE(POUT)((CAPW(I,J),J=1,LL),I=1,LL)
        WRITE(POUT)((CAPV(I,J),J=1,M),I=1,M)
        IF(NTL.GT.0) WRITE(POUT) ((TITLES(I,J),J=1,8),I=1,NTL)
        IF(NTL.GT.0) WRITE(TOUT) ((TITLES(I,J),J=1,8),I=1,NTL)
        WRITE(POUT)NOP,T,ERRLIM,DT
        WRITE(POUT)((CAPMO(I,J),J=1,N),I=1,N)
C
 20     CONTINUE
C
C       THIS IS THE BEGINNING OF LOOP WHICH CALCULATES SYSTEM AND FILTER
C       TIME-HISTORIES WITH THEIR RECURSIVE EQUATIONS.
C       THE LOOP STARTS AT STATEMENT 20 AND ENDS AT 100.
C
C
C       SELECT ERROR CRITERION VALUE ACCORDING TO (LIMIT)...
C
        IF(LIMIT.EQ.1) ERROR = TR (PP,N)
        IF(LIMIT.EQ.2) ERROR = SIGKPN(ZSTAR,PP,N,ND)
C
C       THIS IS THE CRUCIAL CHECK OF MANAGEMENT ALGORITHM...IF THE ERROR
C       IN THE ESTIMATE EXCEEDS THE GIVEN LIMIT, GO TO MAKE A MEASUREMENT.
C       IF NOT, RETURN TO CONTINUE PREDICTION.
C
        IF(ERROR.GE.ERRLIM) GO TO 28
C
C       DO THE OUTPUT FOR TIME T.
C       NOTE...FIRST TIME THROUGH, INITIAL CONDITIONS ARE OUTPUTTED.
C
C       DEFINE THE VARIANCE VECTOR (COV) FROM THE COVARIANCE MATRIX (P)...
        DO  5 I=1,N
  5     COV(I) = PP(I,I)
C
        IF (IOUT(1).NE.-1)
     2  CALL DEBUG (N,L,M,LL,T,TO,X,XH,G,Y,YH,E,W,V,P,PP,IOUT,ND)
C
        IF(IPLT(1).EQ.1) CALL OUTPUT3 (X,3H   X,O,N,T,TO,TI,TST,ST,
     2  XYPW1,XYPW2,TITLES,NTL,NAMEST,NCOLST,IMAX,JMAX,NI,NJ,NK)
        IF(IPLT(2).EQ.1)CALL OUTPUT3 (XHKK,3H XH,O,N,T,TO,TI,TST,ST,
     2  XYPW1,XYPW2,TITLES,NTL,NAMEST,NCOLST,IMAX,JMAX,NI,NJ,NK)
        IF(IPLT(3).EQ.1) CALL OUTPUT3 (E,3H   E,O,N,T,TO,TI,TST,ST,
     2  XYPW1,XYPW2,TITLES,NTL,NAMEST,NCOLST,IMAX,JMAX,NI,NJ,NK)
        IF(IPLT(4).EQ.1) CALL OUTPUT3 (COV,3HCOV,O,N,T,TO,TI,TST,ST,
     2  XYPW1,XYPW2,TITLES,NTL,NAMEST,NCOLST,IMAX,JMAX,NI,NJ,NK)
        IF(IPLT(5).EQ.1) CALL OUTPUT3 (ERROR,SYMBERR(LIMIT),
     1  0,1,T,TO,TI,TST,ST,
     2  XYPW1,XYPW2,TITLES,NTL,NAMEST,NCOLST,IMAX,JMAX,NI,NJ,NK)
C
```

```
C       IF TIME (T) IS AT THE END OF THE INTERVAL (T0,T1), GO TO NEXT RUN.
        IF (T.GE.T1) GO TO 100
C
C       STORE LAST VALUE OF CAVARIANCE IN (P), THEN PREDICTED VALUE IN (PP
C
        CALL ATOB (PP,P,N,N,ND)
        CALL ADOTBT (P,A,W1,N,N,N,ND)
        CALL ADOTB  (A,W1,W3,N,N,N,ND)
        CALL APLUSB (W3,WKP1,PP,N,N,ND)
C
C       OBTAIN INPUT VECTOR OF TIME FUNCTIONS (U(I,T),I=1,L) FOR DETER-
C       MINISTIC FORCING FUNCTION...
        IF(L.NE.0) CALL UBAR(L,T,U,IU,UK,ND)
C
C       GENERATE PROCESS NOISE W(T)...
        CALL NOISEW (T,CAPW,W,SIGMAW,LL,ND)
C
C       INCREMENT TIME (T) AND ITERATION COUNTER (K)
        T = T + DT
        K = K + 1
C
C       CALCULATE MODEL STATE X(K), CALL IT (X)...
C
        DO 24 I=1,N
        X(I) = 0.0
        DO 21 J=1,N
  21    X(I) = X(I) + A(I,J)*XKM1(J)
        IF(L.EQ.0) GO TO 31
        DO 22 J=1,L
  22    X(I) = X(I) + B(I,J)*U(J)
  31    CONTINUE
        DO 23 J=1,LL
  23    X(I) = X(I) + D(I,J)*W(J)
  24    CONTINUE
C       STORE CURRENT (X) IN (XKM1) FOR NEXT ITERATION...
        DO 25 I=1,N
        XKM1(I) = X(I)
  25    CONTINUE
C
C       CALCULATE PREDICTED STATE ESTIMATE XH(K-1,K), CALL IT (XHKM1K)...
C
        DO 39 I=1,N
        XHKM1K(I) = 0.
        DO 36 J=1,N
  36    XHKM1K(I) = XHKM1K(I) + A(I,J)*XHKK(J)
        IF(L.EQ.0) GO TO 32
        DO 37 J=1,L
  37    XHKM1K(I) = XHKM1K(I) + B(I,J)*U(J)
  32    CONTINUE
  39    CONTINUE
C
C       COPY PREDICTED STATE ESTIMATE VECTOR INTO CORRECTED ESTIMATE
C       VECTOR FOR INITIAL VALUE IN NEXT PREDICTED CYCLE...
C
        DO 40 I=1,N
        XHKK(I) = XHKM1K(I)
  40    CONTINUE
C
C       GO TO CHECK FOR VIOLATION OF ESTIMATION ERROR CONSTRAINT...
C
        GO TO 20
C
  28    CONTINUE
C
C       THE ESTIMATION ERROR LIMIT (ERRLIM) HAS BEEN REACHED...
C       IT IS NOW NECESSARY TO TAKE A MEASUREMENT OF THE SYSTEM OUTPUT
C       IN ORDER TO OBTAIN MORE INFORMATION ABOUT THE SYSTEM STATE.
C
C       UNLESS TIME IS AT INITIAL VALUE, BRING BACK TIME TO VALUE WHEN
C       ESTIMATION ERROR WAS LAST SATISFIED IN ORDER TO STORE AND OUTPUT
C       BOTH THE PREDICTED AND CORRECTED VALUES AT EACH MEASUREMENT TIME.
        IF(K.EQ.0) GO TO 29
        T = T - DT
        K = K - 1
  29    CONTINUE
C
C       WRITE NUMBER OF OPTIMIZATION (NOP) AND (P) MATRIX FOR POSTPROCESS
        NOP = NOP + 1
        WRITE(POUT)NOP,T,ERRLIM,DT
        WRITE(POUT)((P(I,J),J=1,N),I=1,N)
C
        WRITE(NOUT,2001)NOP,T
 2001   FORMAT (3H1(X,12,X) SAMPLE, TIME = ,E10.3)
        CALL MATOUTP(P,N,N,1HP,NO)
C
C       (M) IS THE NUMBER OF MEASUREMENTS TO BE TAKEN.  FIND THE OPTIMAL
C       PLACEMENT OF THOSE M MEASUREMENTS, THE PLACEMENT WHICH MINIMIZES
C       THE FUNCTIONAL WHOSE VALUE IS (TR2).  THE OPTIMAL LOCATIONS ARE
C       STORED IN THE VECTOR (Z)...
C
```

```
C      CAUTION ... FIRST TWO ARGUMENTS ARE (M,M2), AS USED HERE, BUT
C      THEY ARE (N,M) AS USED IN (KEELE)...
C
       CALL KEELEA (M,M2,NE,NLIN,FMAX,IW,Z,P11,CONV0,DELT,
     2 EPSLON,RHO,DELTAP,TRPKK,DTRPKK,CONSTR,IFAIL,FLOWER,ACC,IEXP,
     3 NSEARCH)
       IF(ISING.EQ.3) GO TO 994
       IF(IFAIL.GT.0) GO TO 995
       WRITE(POUT)(Z(I),I=1,M)
       CALL KEELEA (M,M2,NE,NLIN,FMAX,IW,Z,P11,CONV0,DELT,
     2 EPSLON,RHO,DELTAP,FVAL,GRADNT,CONSTR,IFAIL,FLOWER,ACC,IEXP,
     3 NSEARCH)
       IF(ISING.EQ.3) GO TO 994
       IF(IFAIL.GT.0) GO TO 995
       WRITE(POUT)(Z(I),I=1,M)
C
C      WITH OPTIMAL MEASUREMENT POSITIONS (Z), CALCULATE
C      OPTIMAL MEASUREMENT MATRIX (C) = (C(Z))...
C
       DO 52 I=1,M
       DO 51 J=1,N
  51   C(I,J) = COS((J-1)*PI*Z(I))
  52   CONTINUE
C
C      KNOWING OPTIMAL PLACEMENT (Z) OF MEASUREMENT DEVICES,
C      CALCULATE MODEL OUTPUT MEASUREMENT Y(K), CALL IT (Y)...
C
C      GET MEASUREMENT NOISE V(T)
       CALL NOISEV (T,CAPV,V,SIGMAV,M,ND)
C
       DO 30 I=1,M
       Y(I) = 0.0
       DO 26 J=1,N
  26   Y(I) = Y(I) + C(I,J)*X(J)
       Y(I) = Y(I) + V(I)
  30   CONTINUE
C
C      CALCULATE FILTER GAIN MATRIX G(K), CALL IT (G)...
C
       CALL ADOTBT (P,C,W1,N,N,M,ND)
       CALL ADOTB  (C,W1,W2,M,N,M,ND)
       CALL APLUSB (W2,CAPV,W1,M,M,ND)
       CALL INVERSE (M,W1,W2,IERR)
       IF (IERR.LT.0) GO TO 992
       CALL ADOTBT (P,C,W3,N,N,M,ND)
       CALL ADOTB  (W3,W2,G,N,M,M,ND)
C
C      CALCULATE CORRECTED STATE ESTIMATE XH(K,K), CALL IT (XHKK)...
C      ALSO CALCULATE ESTIMATE ERROR E(K) = X(K) - XH(K,K), CALL IT (E)..
C
       DO 42 I=1,M
       CXH = 0.0
       DO 41 J=1,N
  41   CXH = CXH + C(I,J)*XHKM1K(J)
       YH(I) = CXH
  42   DY(I) = Y(I) - CXH
       DO 44 I=1,N
       GDY = 0.
       DO 43 J=1,M
  43   GDY = GDY + G(I,J)*DY(J)
       XHKK(I) = XHKM1K(I) + GDY
  44   E(I) = X(I) - XHKK(I)
C
C      CALCULATE CORRECTED ERROR COVARIANCE MATRIX P(K,K), CALL IT (PP)..
C
       CALL ADOTB  (G,C,W1,N,M,N,ND)
       CALL AMINSB (ID,W1,W2,N,N,ND)
       CALL ADOTBT (P,W2,W1,N,N,N,ND)
       CALL ADOTB  (W2,W1,W3,N,N,N,ND)
       CALL ADOTBT (CAPV,G,W1,M,M,N,ND)
       CALL ADOTB  (G,W1,W2,N,M,N,ND)
       CALL APLUSB (W3,W2,PP,N,N,ND)
C
C      FILTER AND STATE CALCULATION FOR THIS STEP IS FINISHED.
C      RETURN TO TOP OF LOOP BETWEEN STMTS 20 AND 100 TO OUTPUT RESULTS,
C      THEN CHECK TIME LIMIT AND CONTINUE SOLUTION.
       GO TO 20
C
 100   CONTINUE
C      THIS IS THE END OF PROBLEM NUMBER (NRUN).  TELL THE TTY AND GO TO
C      NEXT PROBLEM.
       WRITE(NTTY,1001)NRUN
1001   FORMAT(I2,3H OK)
C
C      WRITE (NOP) SET TO ZERO TO CLOSE OUT POSTPROCESSING
       NOP = -1
       WRITE(POUT)NOP,T,ERRLIM,DT
C
       GO TO 1
  99   CONTINUE
```

```
      II = -1
      WRITE(POUT)II
      WRITE(TOUT)II
      CALL  EXIT(0)
C XXX ERROR EXITS XXX
  991 WRITE(NTTY,9991)
 9991 FORMAT(*CANNOT CREATE OUTFILE...TRY AGAIN.*)
      CALL EXIT(0)
  992 WRITE(NOUT,9992)
 9992 FORMAT(/,* SINGULAR MATRIX IN KALMAN GAIN EQUATION.*,/,
     2* OFFENDING MATRIX IS W1 = (CXPXCT + CAPV).*)
      CALL MATOUTP (W1,M,M,2HW1,ND)
C     DUMP OUTPUT GENERATED BEFORE SINGULAR CONDITION OCCURRED.
      CALL OUTPUT3 (X,10H  SINGULAR)
      WRITE(NTTY,9982)NRUN
 9982 FORMAT(I2,8H NG-SING)
C     THIS PROBLEM SINGULAR SO GO TO NEXT PROBLEM IN INPUT DECK...
      GO TO 1
  993 WRITE(NOUT,9993)
 9993 FORMAT(/,*32H THE PAYNTER SERIES EXPANSION CRITERION WAS NOT MET.)
      WRITE(NTTY,9983)NRUN
 9983 FORMAT(I2,8H NG-PAYN)
C     THIS PROBLEM CANNOT BE RUN SO GO TO NEXT ONE IN INPUT DECK...
      GO TO 1
  994 CONTINUE
C     A MATRIX BECAME SINGULAR IN THE OPTIMIZATION PROCEDURE.
C     DUMP OUTPUT BEFORE SINGULAR CONDITION OCCURRED.
      CALL OUTPUT3 (X,10H  SINGULAR)
      WRITE(NTTY,9984)NRUN
 9984 FORMAT(I2,12H NG-SING OPT)
C     THIS PROBLEM SINGULAR SO GO TO NEXT PROBLEM IN INPUT DECK...
      GO TO 1
  995 CONTINUE
C     CONVERGENCE PROBLEMS IN OPTIMIZATION...
      WRITE(NOUT,9995)IFAIL
 9995 FORMAT(/,* CONVERGENCE PROBLEMS IN (KEELEA), IFAIL = *,I2)
      CALL OUTPUT3 (X,10H  SINGULAR)
      WRITE(NTTY,9985)NRUN,IFAIL
 9985 FORMAT(I2,20H NG-CONV OPT, IFAIL=,I2)
      GO TO 1
      END


      SUBROUTINE INPUT (N,L,M,LL,NTL,IPLT,IOUT,LENGTH,
     2 TO,T1,DT,A,B,C,D,IU,UK,
     3 MO,CAPMO,W,CAPW,V,CAPV,IERROR,NOPO,EPS,KMAX,TITLES,ND,
     4 Z,ZU,ZW,ZMAX,ERRLIM,LIMIT,ALPHA,NSEARCH,SYMBERR,
     5 NLIN,FMAX,IW,CONVG,DELT,EPSLON,RHO,DELTAP,FLOWER,ACC,IEXP)
      DIMENSION IPLT(5)
     1          IOUT(10),A(ND,ND),B(ND,ND),C(ND,ND),D(ND,ND),IU(ND),
     2          UK(ND,3),MO(ND),CAPMO(ND,ND),W(ND),CAPW(ND,ND),
     3          V(ND),CAPV(ND,ND),TITLES(4,8),
     4 Z(ND),ZU(ND),ZW(ND)
      DIMENSION SYMBERR(2)
      REAL MO
      COMMON /IO/ NIN,NOUT,NTTY,NRUN,VER
      READ(NIN,101) N,L,M,LL,NTL,(IPLT(I),I=1,5),(IOUT(J),J=1,10),
     2 LENGTH
  101 FORMAT(5I10,5(1X,O1),10I1,I10)
      IF (N.EQ.0) GO TO 991
      IF(NRUN.GT.1) GO TO 1
      IF (LENGTH.EQ.0) LENGTH = 20000
      CALL CREATE (7HOUTFILE,LENGTH,DUMMY)
      IF (DUMMY.LT.0.) GO TO 992
    1 WRITE(NOUT,103)VER,NRUN
      2 N,L,M,LL,NTL,(IPLT(I),I=1,5),(IOUT(J),J=1,10),LENGTH
  103 FORMAT (44H1DISCRETE KALMAN FILTER SIMULATION PROGRAM, ,A10,
     1 10H,  RUN NO. ,I2,
     2 //,31H PROBLEM INPUT IS AS FOLLOWS...//,
     3 10X,3HN,10X,3HL,10X,3HM,9X,2HLL,8X,3HNTL,1X,10H------IPLT,
     4 1X,10H------IOUT,5X,6HLENGTH,/,5(1X,I10),1X,5(1X,O1),1X,10O1,
     5 1X,I10)
C     SEE IF ANY IOUT(I) IS NONZERO.  IF NOT, SET IOUT(1)=-1 AS A FLAG.
C     THIS IS TO SIGNAL THAT (DEBUG) IS NOT USED.  (DEBUG) IS MAINLY
C     USED FOR DEBUGGING PURPOSES ... IT PRODUCES OTHERWISE POOR OUTPUT.
      NDEBUG = 0
      DO 3 I = 1,10
    3 IF(IOUT(I).EQ.1) NDEBUG = NDEBUG + 1
      IF(NDEBUG.EQ.0) IOUT(1) = -1
      READ (NIN,102) TO,T1,DT,NOPO,EPS,KMAX
  102 FO.MAT (3E10.3,I10,E10.3,I10)
      IF (EPS.EQ.0.0) EPS = 1.E-5
      IF(KMAX.EQ.0) KMAX = 100
      WRITE(NOUT,105) TO,T1,DT,NOPO,EPS,KMAX
  105 FORMAT(/,9X,2HTO,9X,2HT1,9X,2HDT,7X,4HNOPO,8X,3HEPS,7X,4HKMAX,/,
     2 3(1X,E10.3),1X,I10,1X,E10.3,1X,I10,/)
      T1 = .09999999 + T1
      READ(NIN,120)NLIN,FMAX,IW,IEXP,CONVG,DELT,EPSLON,RHO,DELTAP,
     2           FLOWER,ACC
  120 FORMAT(4I10,/,7E10.9)
```

```
      IF (NTL.EQ.0) GO TO 5
      DO 2 I=1,NTL
      READ (NIN,100) (TITLES(I,J),J=1,8)
100   FORMAT(8A10)
      WRITE (NOUT,108) (TITLES(I,J),J=1,8)
108   FORMAT(1X,8A10)
2     CONTINUE
5     CONTINUE
      IF(L.EQ.0) GO TO 7
      WRITE (NOUT,106)
106   FORMAT(/,* INPUT SELECTORS AND PARAMETER VALUES ARE AS FOLLOWS...*
     2 /,*  I   INPT        A(1)        A(2)        A(3)*)
      DO 10 I=1,L
      READ (NIN,104) IU(I),(UK(I,J),J=1,3)
104   FORMAT (I1,9X,7E10.3)
      WRITE (NOUT,107) I,IU(I),(UK(I,J),J=1,3)
107   FORMAT (I3,I6,7(1X,E10.3))
10    CONTINUE
7     CONTINUE
      CALL VECINPT (M0,N,2HM0,ND)
      CALL MATINPT (CAPM0,N,N,5HCAPM0,ND)
      CALL MATINPT (CAPW,LL,LL,4HCAPW,ND)
      CALL MATINPT (CAPV,M,M,4HCAPV,ND)
C
C     PROBLEM STRUCTURE IS FORMULATED IN DIMENSIONLESS COORDINATES
C     SO THAT ONE-DIMENSIONAL MEDIUM IS OF UNIT LENGTH...
      ZMAX = 1.0
C
      IF(L.NE.0) CALL VECINPT (ZU,L,2HZU,ND)
      CALL VECINPT (ZW,LL,2HZW,ND)
      CALL VECINPT(Z,M,1HZ,ND)
      READ(NIN,111) ERRLIM,LIMIT,ALPHA,NSEARCH
111   FORMAT(2(E10.3,I10))
      WRITE(NOUT,112) NSEARCH
112   FORMAT (//,
     3 6CH NUMBER OF POINTS FOR RANDOM SEARCH INITIALIZATION (NSEARCH) =
     4 I5)
      IF(LIMIT.EQ.1) WRITE(NOUT,113)ERRLIM
113   FORMAT(//,* THIS IS A MONITORING PROBLEM OF THE FIRST KIND=*,/,
     2 * WITH A CONSTRAINT ON THE ALLOWABLE ERROR IN THE STATE ESTIMATE=
     3 ,/,* THE ESTIMATION ERROR CRITERION IS THE TRACE(P(K,K+N))=*,//,
     4 * THE CONSTRAINT ON THE ERROR IN THE STATE ESTIMATE IS FIXED AT=,
     5 /,* TRLIM =*,E10.3,/,*I*)
      IF(LIMIT.EQ.2)WRITE(NOUT,114)ERRLIM
114   FORMAT(//,* THIS IS A MONITORING PROBLEM OF THE SECOND KIND=*,/,
     2* WITH A CONSTRAINT ON THE ALLOWABLE ERROR IN THE OUTPUT=*,
     3 * ESTIMATE*,/,* THE ESTIMATION ERROR CRITERION IS THE MAXIMUM=*,
     4 * VALUE OVER THE LENGTH OF THE MEDIUM Z*,/,
     5 * OF THE VARIANCE OF THE ESTIMATE OF THE OUTPUT GIVEN BY...=*,/,
     6 *       SIGMA(Z) = C(Z) . [P(K,K+N)] . C(Z)=*,/,
     7 * THE CONSTRAINT IN THE ERROR IN THE OUTPUT ESTIMATE IS FIXED=*,
     8 * AT=,//,* SIGMALIM =*,E10.3,/,*I*)
      WRITE(NOUT,110) ALPHA
110   FORMAT(//,*PARAMETERS FOR SYSTEM DESCRIPTION ARE...=*,//,
     2 * DIFFUSION CONSTANT  K =  1.000E+00=*,/,
     3 * LENGTH OF MEDIUM    L =  1.000E+00=*,/,
     4 * SCAVENGING RATE ALPHA = *,E10.3)
C     KNOWING ZU AND ZW VECTORS, DEFINE SYSTEM MATRICES A,B AND D...
      PI = 3.14159265
      DO 12 I=1,N
      DO 11 J=1,N
      A(I,J) = 0.
11    A(I,I) = -(((I-1)*PI)**2 + ALPHA)
12    DO 15 I=1,N
      IF(L.EQ.0) GO TO 8
      DO 13 J=1,L
      B(I,J) = COS((I-1)*PI*ZU(J))
13    IF(I.EQ.1) B(I,J) = .5
8     CONTINUE
      DO 14 J=1,LL
      D(I,J) = COS((I-1)*PI*ZW(J))
14    IF(I.EQ.1) D(I,J) = .5
15    CONTINUE
      CALL MATOUTP (A,N,N,1HA,ND)
      IF (L.NE.0) CALL MATOUTP (B,N,L,1HB,ND)
      CALL MATOUTP (D,N,LL,1HD,ND)
      IERROR = 0
      RETURN
C     ERROR EXITS...
C     IERROR = 0, OK.
C     IERROR = -1, END OF INPUT DECK, RETURN TO EXIT.
C     IERROR = -2, CANNOT CREATE OUTPUT FILE, RETURN TO EXIT.
 991  IERROR = -1
      RETURN
 992  IERROR = -2
      RETURN
      END


      SUBROUTINE FVAL (Z,P11)
```

```
C       RETURNS [P(K,K)(Z(K))](1,1)...
C       FOR USE IN MAXIMIZATION OF ERROR-LIMIT INTERCEPT TIME BY
C       MINIMIZING THE (1,1) ELEMENT OF THE CORRECTED COVARIANCE MATRIX
C       AT TIME (K).
        COMMON /PROB/ N,M,ZMAX,A,P,CAPV,WKP1,WSS,ISING
        DIMENSION A(10,10),P(10,10),CAPV(10,10),WKP1(10,10),WSS(10,10)
        DIMENSION C(10,10),PSII(10,10),Z(1),W1(10,10),W2(10,10),W3(10,10)
        ND = 10
        PI = 3.14159266
        DO 12 I=1,M
        DO 11 J=1,N
11      C(I,J) = COS((J-1)*PI*Z(I))
12      CONTINUE
C       FIRST COMPUTE [PSII] == [C*P(K-1,K)*CT]INVERSE...
        DO 5 IA=1,M
        DO 2 IC=1,N
        W1(IA,IC) = 0.
        DO 1 ID=1,N
1       W1(IA,IC) = W1(IA,IC) + C(IA,ID)*P(ID,IC)
2       CONTINUE
        DO 4 IB=1,M
        W2(IA,IB) = CAPV(IA,IB)
        DO 3 IE=1,N
3       W2(IA,IB) = W2(IA,IB) + W1(IA,IE)*C(IB,IE)
4       CONTINUE
5       CONTINUE
        CALL INVERSE (M,W2,PSII,IERR)
        IF(IERR.LT.0) GO TO 991
C       COMPUTATION OF [P(ZK)(K,K)]11...
        P11 = P(1,1)
        DO 7 IC=1,M
        W1PI = 0.
        DO 6 ID=1,M
6       W1PI = W1PI + W1(ID,1)*PSII(ID,IC)
7       P11 = P11 - W1PI*W1(IC,1)
        ISING = 0
99      RETURN
991     ISING = 3
        RETURN
        END


        SUBROUTINE GRADNT (Z,DP11)
C
C       RETURNS D[P(K,K)(Z(K))](1,1)/DZ...
C       THE DERIVATIVE IF THE (1,1) ELEMENT OF THE CORRECTED COVARIANCE
C       MATRIX AT TIME (K) WITH RESPECT TO THE VECTOR (Z(K)).
C
        COMMON /PROB/ N,M,ZMAX,A,P,CAPV,WKP1,WSS,ISING
        DIMENSION A(10,10),P(10,10),CAPV(10,10),WKP1(10,10),WSS(10,10)
        DIMENSION C(10,10),DC(10,10),Z(1),DP11(1),W1(10,10),W2(10,10),
     2  W3(10,10),PSII(10,10)
        ND = 10
        PI = 3.14159266
C
C       FIRST COMPUTE [PSII] == [C*P(K-1,K)*CT]INVERSE...
C
C       GENERATE C(Z(K)) MATRIX (CALL IT C)...
C       GENERATE DC(I,J)/DZ(I) MATRIX (CALL IT DC)...
        DO 20 I=1,M
        DO 19 J=1,N
        C(I,J) =                    COS((J-1)*PI*Z(I))
19      DC(I,J) = -(J-1)*PI*SIN((J-1)*PI*Z(I))
20      CONTINUE
C
        DO 5 IA=1,M
        DO 2 IC=1,N
        W1(IA,IC) = 0.
        DO 1 ID=1,N
1       W1(IA,IC) = W1(IA,IC) + C(IA,ID)*P(ID,IC)
2       CONTINUE
        DO 4 IB=1,M
        W2(IA,IB) = CAPV(IA,IB)
        DO 3 IE=1,N
3       W2(IA,IB) = W2(IA,IB) + W1(IA,IE)*C(IB,IE)
4       CONTINUE
5       CONTINUE
        CALL INVERSE (M,W2,PSII,IERR)
        IF(IERR.LT.0) GO TO 991
C
C       COMPUTE PSII*C*P...
C
        DO 7 IA=1,M
        W2(IA,1) = 0.
        DO 6 IB=1,M
6       W2(IA,1) = W2(IA,1) + PSII(IA,IB)*W1(IB,1)
7       CONTINUE
C
C       COMPUTE BRACKETED MIDDLE TERM OF SECOND MATRIX EXPRESSION...
C
```

```
      DO 12 IA=1,M
      DO 11 IC=1,M
      W3(IA,IC) = 0.
      DO 10 IB=1,N
   10 W3(IA,IC) = W3(IA,IC) + W1(IA,IB)*DC(IC,IB)
   11 CONTINUE
   12 CONTINUE
C
C     NOW COMPUTE THREE MATRIX TERMS IN GRADIENT...
C     FIRST TERM...
C
      DO 89 II=1,M
C
      DP11(II) = 0.
C
      PDC = 0.
      DO 8 IA=1,N
    8 PDC = PDC + P(1,IA)*DC(II,IA)
      DP11(II) = PDC*W2(II,1)
C
C     THIRD TERM EQUALS FIRST TERM, SO JUST DOUBLE THE FIRST...
C
      DP11(II) = 2.*DP11(II)
C
C     FINALLY, COMPLETE SECOND TERM...
C
      DO 24 IB=1,M
      IF(IB.EQ.II) GO TO 22
      PDCP = W2(II,1)*W3(IB,II)
      GO TO 24
   22 PDCP = W2(II,1)*W3(II,II)
      DO 23 IA=1,M
   23 PDCP = PDCP + W2(IA,1)*W3(IA,II)
   24 DP11(II) = DP11(II) - PDCP*W2(IB,1)
C
C     INCLUDE OVERALL MINUS SIGN
C
      DP11(II) = -1.*DP11(II)
C
   89 CONTINUE
   90 ISING = 0
      RETURN
  991 ISING = 3
      RETURN
      END


      SUBROUTINE CONSTR
      COMMON /BAMRWH/ G(10,20),B(20)
      DIMENSION A(10,10),P(10,10),CAPV(10,10),WKP1(10,10),WSS(10,10)
      COMMON /PROB/ N,M,ZMAX,A,P,CAPV,WKP1,WSS,ISING
      DO 1 I=1,M
      G(I,I) = -1.
      B(I) = 0.
      G(I,M+I) = 1.
    1 B(M+I) = ZMAX
      RETURN
      END


      SUBROUTINE TRPKK (Z,TRP)
      COMMON /PROB/ N,M,ZMAX,A,P,CAPV,WKP1,WSS,ISING
      DIMENSION A(10,10),WKP1(10,10),WSS(10,10)
      DIMENSION P(10,10),C(10,10),CAPV(10,10),PSI(10,10)
      DIMENSION Z(1),W1(10,10),W2(10,10),W3(10,10)
      ND = 10
      PI = 3.14159268
C     CALCULATE C(Z) AND PSI((C(Z)) AND PUT IN COMMON...
      DO 2 I=1,M
      DO 1 J=1,N
    1 C(I,J) = COS((J-1)*PI*Z(I))
    2 CONTINUE
      CALL ADDTB  (C,P,W1,M,N,N,ND)
      CALL ADDTBT (W1,C,W2,M,N,M,ND)
      CALL APLUSB (W2,CAPV,W3,M,M,ND)
      CALL INVERSE (M,W3,PSI,IERR)
      IF(IERR.LT.0)GO TO 991
      CALL ADDTB  (PSI,W1,W2,M,M,N,ND)
      CALL ATDOTB (W1,W2,W3,N,M,N,ND)
      CALL AMINSB (P,W3,W2,N,N,ND)
      TRP = 0.
      DO 10 I=1,N
   10 TRP = TRP + W2(I,I)
      ISING = 0
   99 RETURN
  991 ISING = 3
      RETURN
      END
```

```
      SUBROUTINE DTRPKK (Z,DDZ)
      COMMON /PROB/ N,M,ZMAX,A,P,CAPV,WKP1,WSS,ISING
      DIMENSION A(10,10),WKP1(10,10),WSS(10,10)
      DIMENSION P(10,10),C(10,10),CAPV(10,10),PSII(10,10)
      DIMENSION Z(1),DDZTRP(1),W1(10,10),W2(10,10)
     2 W3(10,10 ),W4(10,10),W5(10,10),W6(10,10),DC(10,10)
      ND = 10
      PI = 3.14159266
C     GENERATE C...
      DO 10 I=1,M
      DO  9 J=1,N
    9 C(I,J) = COS((J-1)*PI*Z(I))
   10 CONTINUE
C     FIND PSII = PSI INVERSE
      CALL ADDTB  (C,P,W1,M,N,N,ND)
      CALL ADDTBT (W1,C,W2,M,N,M,ND)
      CALL APLUSB (W2,CAPV,W3,M,M,ND)
      CALL INVERSE (M,W3,PSII,IERR)
      IF(IERR.LT.0)GO TO 991
      CALL ADDTB  (PSII,W1,W2,M,M,N,ND)
      DO 89 II = 1,M
C     GENERATE DC(I,J)/DZ(I) MATRIX (CALL IT DC)...
      DO 6 I=1,M
      DO 5 J=1,N
    5 DC(I,J) = 0.
    6 CONTINUE
      DO 7 J=1,N
    7 DC(II,J) = -(J-1)*PI*SIN((J-1)*PI*Z(II))
C     NOW CALCULATE THREE MATRIX TERMS, FIRST TERM (W4)...
      CALL ATDOTB (DC,W2,W3,N,M,N,ND)
      CALL ADDTB  (P,W3,W4,N,N,N,ND)
C     SECOND TERM (W5)...
      CALL ADDTBT (W1,DC,W3,M,N,M,ND)
      CALL APLUSB (W3,W3,W5,M,M,ND)
      CALL ADDTB  (W5,W2,W6,M,M,N,ND)
      CALL ATDOTB (W2,W6,W5,N,M,N,ND)
C     THIRD TERM, NOTE, THIRD TERM = (FIRST TERM)T, SO JUST ADD UP TERMS
      CALL AMINSB (W4,W5,W6,N,N,ND)
      CALL APLUSBT(W6,W4,W5,N,N,ND)
      DDZTRP(II) = 0.
      DO 12 I=1,N
   12 DDZTRP(II) = DDZTRP(II) - W5(I,I)
   89 CONTINUE
   90 ISING = 0
      RETURN
  991 ISING = 3
      RETURN
      END


      FUNCTION SIGKPN (ZSTAR,PP,N,ND)
C     FINDS...
C         SIGMA**2(ZK,ZSTAR) = C(ZSTAR)T * PP(ZK)(K,K+N) * C(ZSTAR)
      DIMENSION C(10),PP(10,10)
      PI = 3.14159266
      DO 1 I=1,N
    1 C(I) = COS((I-1)*PI*ZSTAR)
      CALL XTAY (C,PP,C,SIGKPN,N,ND)
      RETURN
      END


      FUNCTION SIGMA(Z)
      COMMON /PROB/ N,M,ZMAX,A,P,CAPV,WKP1,WSS,ISING
      DIMENSION A(10,10),P(10,10),CAPV(10,10),WKP1(10,10),WSS(10,10)
      DIMENSION C(10)
      PI = 3.14159266
      DO 1 J=1,N
    1 C(J) = COS((J-1)*PI*Z)
      CALL XTAY (C,WSS,C,SIGMA,N,10)
      RETURN
      END


      FUNCTION DSIGMA(Z)
      COMMON /PROB/ N,M,ZMAX,A,P,CAPV,WKP1,WSS,ISING
      DIMENSION A(10,10),P(10,10),CAPV(10,10),WKP1(10,10),WSS(10,10)
      DIMENSION C(10),DC(10)
      PI = 3.14159266
      DO 1 J=1,N
        C(J) =                COS((J-1)*PI*Z)
    1 DC(J) = -(J-1)*PI*SIN((J-1)*PI*Z)
      CALL XTAY (DC,WSS,C,TERM,N,10)
      DSIGMA = 2.*TERM
      RETURN
      END


      SUBROUTINE SS (N,A,WKP1,EPS,NSS,WSS,ND)
C     FIND (NSS), THE POWER TO WHICH (A) MUST BE RAISED BEFORE
```

```
      (A(2,2)**NSS/A(2,2)).LT.EPS...
      DIMENSION A(10,10),WKP1(10,10),WSS(10,10),
     2 W1(10,10),W2(10,10),SUM(10,10)
      NSS = 1
    1 NSS = NSS+1
      RATIO = A(2,2)**NSS/A(2,2)
      IF(RATIO.LE.EPS) GO TO 2
      GO TO 1
    2 CONTINUE
C     FIND (WSS), STEADY-STATE MATRIX CONVOLUTION OF (WKP1)...
      CALL ATOB (WKP1,W2,N,N,ND)
      CALL ATOB (WKP1,SUM,N,N,ND)
      DO 7 K=1,NSS
      CALL ATOB (W2,W1,N,N,ND)
      CALL ABAT (A,W1,W2,N,ND)
      CALL APLUSB (SUM,W2,SUM,N,N,ND)
    7 CONTINUE
      CALL ATOB (SUM,WSS,N,N,ND)
      CALL MATOUTP (WSS,N,N,3HWSS,ND)
      WRITE(3,108)NSS
  108 FORMAT(/,* THE NUMBER OF TERMS IN THE TRUNCATED MATRIX*,
     1 * CONVOLUTION SERIES*,/,
     2* FOR THE STEADY-STATE VALUE OF (WSS) NSS = *,I3)
      RETURN
      END


      SUBROUTINE MAXSIG (SIGMAX,YSTAR,G,EPS,ITER)
      EXTERNAL DSIGMA,SIGMA
      YMIN = 0.
      YMAX = 1.
      DY = G*(YMAX-YMIN)
      YL = YMIN
      YR = YMIN+DY
      SUP = SIGMA(YL)
      YSUP = YL
      IEND = ITER
    1 CONTINUE
      CALL MUELLER (Y,FY,DSIGMA,YL,YR,EPS,IEND,IER)
C     FINISHED WITH CURRENT INTERVAL.  SLIDE LIMITS OF SEARCH RIGHT
C     CHECK FOR BOUNDARY AND GO ON...
      IF(IER.GT.0) GO TO 13
C     IF AN EXTREMUM WAS FOUND IN THIS INTERVAL, CHECK IT AGAINST LAST
C     VALUE OF SUPREMUM...
      FMUEL = SIGMA(Y)
      IF(FMUEL.LT.SUP) GO TO 11
      SUP = FMUEL
      YSUP = Y
   11 CONTINUE
   13 CONTINUE
      YL = YR
      YR = YR+DY
      IF(YR.GT.YMAX) GO TO 20
      FR = SIGMA(YR)
      IF(FR.LT.SUP) GO TO 12
      SUP = FR
      YSUP = YR
   12 CONTINUE
      GO TO 1
   20 CONTINUE
C     INTERVAL (YMIN,YMAX) HAS BEEN SEARCHED...
      SIGMAX = SUP
      DSIGMAX = DSIGMA(YSUP)
      YSTAR = YSUP
      WRITE(3,101)YMIN,YMAX,G,SIGMAX,DSIGMAX,YSTAR
  101 FORMAT (/,* MAXIMUM SIGMA SOUGHT BETWEEN YMIN = *,E10.3,
     2 /,* AND YMAX = *,E10.3,* WITH INTERVAL WIDTH DY = *,E10.3,/,
     3 * SIGMAX = *,E10.3,*, DSIGMAX = *,E10.3,*, YSTAR = *,E10.3)
      RETURN
      END


      SUBROUTINE MUELLER (X,F,FCT,XLI,XRI,EPS,IEND,IER)
C
C     REF...IBM SCIENTIFIC SUBROUTINE SUBROUTINE PACKAGE,
C     SUBROUTINE RTMI, IBM SSP PROGRAMMERS MANUAL, EDITION 4, 1968,
C     P. 217.
C
      IER=0
      XL=XLI
      XR=XRI
      X=XL
      TOL=X
      F=FCT(TOL)
      IF(F)1,16,1
    1 FL=F
      X=XR
      TOL=X
      F=FCT(TOL)
      IF(F)2,16,2
```

```
      2     FR=F
      C     CHECK FL*FR .LT. 0.
            IF(SIGN(1.,FL)+SIGN(1.,FR))25,3,25
      3     I=0
            TOLF=100.*EPS
      4     I=I+1
            DO 13 K=1,IEND
            X=.5*(XL+XR)
            TOL=X
            F=FCT(TOL)
            IF(F)5,16,5
      5     IF(SIGN(1.,F)+SIGN(1.,FR))7,6,7
      6     TOL=XL
            XL=XR
            XR=TOL
            TOL=FL
            FL=FR
            FR=TOL
      7     TOL=F-FL
            A=F*TOL
            A=A+A
            IF(A-FR*(FR-FL))8,9,9
      8     IF(I-IEND)17,17,9
      9     XR=X
            FR=F
            TOL=EPS
            A=ABS(XR)
            IF(A-1.)11,11,10
     10     TOL=TOL*A
     11     IF(ABS(XR-XL)-TOL)12,12,13
     12     IF(ABS(FR-FL)-TOLF)14,14,13
     13     CONTINUE
      C     END OF BISECTION.
      C     ERROR RETURN...NO CONVERGENCE WITHIN (IEND) ITERATIONS
            IER=1
     14     IF(ABS(FR)-ABS(FL))16,16,15
      C     NORMAL RETURN
     15     X=XL
            F=FL
     16     RETURN
      C     ITERATED INVERSE PARABOLIC INTERPOLATION...
     17     A=FR-F
            DX=(X-XL)*FL*(1.+F*(A-TOL)/(A*(FR-FL)))/TOL
            XM=X
            FM=F
            X=XL-DX
            TOL=X
            F=FCT(TOL)
            IF(F)18,16,18
     18     TOL=EPS
            A=ABS(X)
            IF(A-1.)20,20,19
     19     TOL=TOL*A
     20     IF(ABS(DX)-TOL)21,21,22
     21     IF(ABS(F)-TOLF)16,16,22
     22     IF(SIGN(1.,F)+SIGN(1.,FL))24,23,24
     23     XR=X
            FR=F
            GO TO 4
     24     XL=X
            FL=F
            XR=XM
            FR=FM
            GO TO 4
      C     ERROR...WRONG INPUT DATA
     25     IER=2
            RETURN
            END


            SUBROUTINE KEELEA (N,M,NE,NLIN,FMAX,IW,XINF,FINF,CONVG,DELT,
           2 EPSLON,RHO,DELTAP,FVAL,GRADNT,CONSTR,IFAIL,FLOWER,ACC,IEXP,
           3 NSEARCH)
      C     VERSION (A) OF (KEELE).  (NSEARCH) MINIMIZATIONS ARE ATTEMPTED
      C     EACH FROM A DIFFERENT RANDOM VECTOR WHOSE ELEMENTS ARE SCALED
      C     TO LIE WITHIN 0.LE.Z(I).LE.ZMAX.
            DIMENSION S(10,10),GTSG(20,20),P(20),PAR(20),PL(20),PA(20)
            DIMENSION XB(10),EXTRA(10)
            DIMENSION XINF(10)
            ZMAX = 1.
            REAL NORM,NORM1,NORM2
            INTEGER COL(20),DEPC(20),FNUM,FMAX,COL1,COLJ
            COMMON /BAMRWH/ G(10,20),B(20)
      C  REFERENCE...
      C
      C  PROGRAM AUTHOR  G. W. WESTLEY
      C  COMPUTING TECHNOLOGY CENTER  UNION CARBIDE CORP.
      C  NUCLEAR DIVISION
      C  OAK RIDGE, TENN.
      C
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```
C
C     MODIFIED TO RUN AT LLL 7/25/72 BY R.F.HAUSMAN,JR
C
C      IV IS THE MAXIMUM NUMBER OF VARIBLES ALLOWED.
C      IC IS THE MAXIMUM NUMBER OF CONSTRAINTS ALLOWED.
C
C     IO1 IS THE LOGICAL UNIT NUMBER FOR PRINTOUT
C
      IV = 10
      IC = 20
      IO1 = 3
C
      LABEL1 = 6H  CONV
      LABEL2 = 10HERGENCE **
      LBLMAX = N + 1
      IF(LBLMAX.GT.7) LBLMAX = 7
C
      TOL1 = 1.E-10
      IF (IW.GT.0) WRITE(IO1,1040 ) N,M,NE,IEXP,NLIN,FMAX,IW,CONVG,DELT,
     > EPSLON,RHO,DELTAP,TOL
      IF(IW.EQ.2)WRITE(IO1,1049)
      ISEARCH = 0
      DO 1 I=1,N
    1 XB(I) = XINF(I)
      CALL FVAL (XINF,FINF)
      IF(NSEARCH.EQ.0) GO TO 5
      NSEARP1 = NSEARCH + 1
    2 ISEARCH = ISEARCH + 1
      IF(ISEARCH.EQ.1) GO TO 5
      IF(ISEARCH.GT.NSEARP1)GO TO 798
      ISEARM1 = ISEARCH - 1
      WRITE(IO1,1048)ISEARM1
C     GENERATE A NEW RANDOM STARTING VECTOR...
      DO 3 I=1,N
    3 XB(I) = ZMAX*RAND(IY)
    5 CONTINUE
      IFAIL = 0
      ILAST = 0
      NBC = 0
      FNUM = 0
      IFRST = 0
      NDEP = 0
      NDEPEQ = 0
      FNUM = FNUM + 1
      CALL FVAL(XB,FB)
      IF((IW.GT.0).AND.(IW.NE.2))
     2          WRITE(IO1,1050 ) FNUM,FB,(XB(I),I=1,N)
      IF(IW.EQ.2)WRITE(IO1,1051)FNUM,FB,(XB(I),I=1,N)
C
C      SET THE INITIAL S TO I.
      DO 20 I=1,N
         DO 10 J=1,N
   10       S(I,J) = 0.
   20    S(I,I) = 1.
      IF (M.EQ.0) GO TO 90
C
C      ZERO OUT THE COEFFICIENT MATRIX.
C
      DO 30 J=1,M
         COL(J) = 0
         DEPC(J) = 0
         B(J) = 0.0
         DO 30 I=1,N
   30       G(I,J) = 0.
C
C      INITALIZE THE NON-ZERO COEFFICIENTS IN THE CONSTRAINTS.
C      THIS IS SUPPLIED IN THE ROUTINE CONSTR BY THE USER.
C
      CALL CONSTR
C
C
C
C      ADJUST THE CONSTRAINTS TO UNIT NORM.
C      G IS THE COEFFICIENT MATRIX       G(1,1)*X(1)  +  G(2,1)*X(2)  +
C      B IS THE VECTOR OF CONSTRAINT CONSTANTS,
C
      DO 60 J=1,M
         SUM = 0.
         DO 40 I=1,N
   40       SUM = SUM + G(I,J)*G(I,J)
      SUM = SQRT(SUM)
         DO 50 I=1,N
   50       G(I,J) = G(I,J)/SUM
   60    B(J) = B(J)/SUM
C
C
      NE1 = NE + 1
      NE2 = NE + 2
      IF (NE.EQ.0) GO TO 90
      I = 1
```

```
      CALL CONADD(GTSG,S,I,COL,P,PL,N,NBC,IV,IC)
      IF (IW.GE.2) WRITE(101,1110 ) I,NBC
      IF (NE.EQ.1) GO TO 90
      DO 80 I=2,NE
C
C       PROJECT THE I-TH CONSTRAINT TO TEST FOR LINEAR INDEPENDENCE.
C
         CALL PROJCT(PL,P,EXTRA,S,GTSG,N,NBC,COL,I,IV,IC, NORM1)
         IF (IW.GT.2) WRITE(101,1120 ) I,NORM1,TOL1
C
C       TEST AGAINST TOL1 FOR LINEAR DEPENDENCE
C
         IF (NORM1.GT.TOL1) GO TO 70
         NDEP = NDEP + 1
         NDEPEQ = NDEP
         DEPC(NDEP) = I
         GO TO 80
   70    CALL CONADD(GTSG,S,I,COL,P,PL,N,NBC,IV,IC)
         IF (IW.GE.2) WRITE(101,1110 ) I,NBC
   80    CONTINUE
      NE1 = NE - NDEPEQ + 1
      NE2 = NE1 + 1
C
C
C       CALCULATE THE PARTIAL VECTOR OF THE OBJECTIVE FUNCTION.
C
   90 CALL GRADNT(XB,PAR)
C
C       GENERATE THE SEARCH DIRECTION.
C
  100 CONTINUE
      DO 110 I=1,N
  110    PA(I) = -PAR(I)
C
C       IF THERE ARE CONSTRAINTS IN THE BASIS THEN CALCULATE THE PROJECTI
C
      IF (NBC.EQ.0) GO TO 170
      DO 120 I=1,N
         PL(I) = 0.
         DO 120 J=1,N
  120       PL(I) = PL(I) + S(I,J)*PAR(J)
C
C       COL(I) = K   IMPLIES THAT THE K-TH CONSTRAINT IS IN COL I OF BASI
C
      DO 130 I=1,NBC
         PA(I) = 0.
         LA = COL(I)
         DO 130 J=1,N
  130       PA(I) = PA(I) + G(J,LA)*PL(J)
C
C       PUT THE LAGRANGE VECTOR IN THE VECTOR PL.
CC
      DO 140 I=1,NBC
         PL(I) = 0.
         DO 140 J=1,NBC
  140       PL(I) = PL(I) + GTSG(I,J)*PA(J)
C
C
      DO 150 I=1,N
         PA(I) = 0.
         DO 150 J=1,NBC
            COLJ = COL(J)
  150       PA(I) = PA(I) + G(I,COLJ  )*PL(J)
      DO 160 I=1,N
  160    PA(I) = PA(I) - PAR(I)
C
C
  170 CONTINUE
C
C
C       PA HOLDS THE INFO FOR THE DOWNHILL-POSITIVE DEFINITE CHECK.
C
C       P HOLDS THE SEARCH DIRECTION.
C
      DO 180 I=1,N
         P(I) = 0.
         DO 180 J=1,N
  180       P(I) = P(I) + S(I,J) * PA(J)
C
C
C
C       FIND THE NORM OF THE DIRECTION VECTOR.
C
      NORM1 = 0.
      NORM = 0.
      DO 190 I=1,N
         NORM1 = NORM1 + PA(I)**2
  190    NORM = NORM + P(I)**2
      NORM = SQRT(NORM)
```

```
1145          NORM1 = SQRT(NORM1)
1146          NORM2 = NORM
1147          BETA = 0.
1148          J = 0
1149          IF (NBC.EQ.(NE-NDEPEQ)) GO TO 220
1150    C
1151    C
1152    C      CALCULATE THE LAGRANGE MULTIPLIER VECTOR ON THOSE INEQUALITY
1153    C      CONSTRAINTS IN THE BASIS.
1154    C
1155          J = NE1
1156          CC = PL(NE1)
1157          IF (NBC.EQ.NE1) GO TO 210
1158          DO 200 I=NE2,NBC
1159             IF (PL(I).LE.CC) GO TO 200
1160             J = I
1161             CC = PL(I)
1162      200    CONTINUE
1163      210 BETA = .5*CC/ABS(GTSG(J,J))
1164      220 CONTINUE
1165          IF (IW.GT.2) WRITE(101,1010 ) NORM,BETA,J
1166          IF (NORM.LE.CONVG.AND.BETA.LE.CONVG) GO TO 710
1167    C
1168    C
1169    C      THE PROCEDURE HAS NOT CONVERGED YET.  EITHER DROP THE J-TH COL.
1170    C      OF THE BASIS AND RE-CHECK OR STEP ALONG  THE DIRECTION IN P.
1171    C
1172    C
1173          IF (NORM.GT.BETA) GO TO 250
1174    C
1175    C      DROP THE CONSTRAINT CORRESPONDING TO MAXIMUM LAGRANGE.
1176    C
1177    C
1178    C      SINCE A CONSTRAINT IS BEING DROPPED    -     FORGET ABOUT ALL OF TH
1179    C      PREVIOUS INEQUALITY DEPENDENCE.
1180    C
1181          IF (NDEP.EQ.0) GO TO 240
1182          K = NDEPEQ + 1
1183          DO 230 I=K,NDEP
1184      230    DEPC(I) = 0
1185          NDEP = NDEPEQ
1186      240 ILAST = COL(J)
1187          IF (IW.GT.2) WRITE(101,1080 ) ILAST
1188          CALL CONDRP(COL,J,NBC,GTSG,PL,IC)
1189          GO TO 100
1190    C
1191    C
1192    C      THERE ARE NO CONSTRAINTS TO DROP FROM THE BASIS SO EXAMINE THE
1193    C      DIRECTION FOR IMPROVEMENT.
1194    C
1195    C
1196      250 CONTINUE
1197          LL = 0
1198          CC = 1.E+60
1199          IF ((NBC+NDEP).EQ.M) GO TO 320
1200          DO 310 I=1,M
1201             IF (ILAST.EQ.I) GO TO 310
1202             IF (NBC.EQ.0) GO TO 280
1203             DO 260 K=1,NBC
1204                IF (I.EQ.COL(K)) GO TO 310
1205      260    CONTINUE
1206             IF (NDEP.EQ.0) GO TO 280
1207             DO 270 K=1,NDEP
1208                IF (I.EQ.DEPC(K)) GO TO 310
1209      270    CONTINUE
1210    C
1211    C       CONSTRAINT I IS NOT IN THE BASIS.  IS IT BINDING.....
1212    C
1213      280    CON1 = B(I)
1214             CON2 = 0.
1215             DO 290 J=1,N
1216                CON1 = CON1 - XB(J)*G(J,I)
1217      290       CON2 = CON2 + P(J)*G(J,I)
1218          IF(IW.EQ.3)WRITE(101,1000 ) I,CON1,CON2
1219             IF (CON2.EQ.0.   ) GO TO 310
1220          NORM = ABS(CON1)
1221             IF (NORM.GT.1.E-14) GO TO 300
1222             IF (CON2.GT.0.   ) GO TO 700
1223             GO TO 310
1224      300    CON1 = CON1/CON2
1225          IF(CON1.LE.0.E+00.OR.CON1.GE.CC) GO TO 310
1226             CC=CON1
1227             LL=I
1228      310    CONTINUE
1229    C 320 NORM = DMIN1(1.D0,CC)
1230      320 NORM = CC
1231          IF(NORM.GT.1.) NORM = 1.
1232          ILAST = 0
1233    C
1234    C       CALCULATE THE INDEX OF IMPROVEMENT-----CON2.
```

```
C       IMPROVEMENT IS ACCEPTED IF F(K) - F(K+1) .GE. EPSLON * CON2.
C
      CON2 = 0.
      DO 330 I=1,N
  330    CON2 = CON2 - PAR(I)*P(I)
      IF (IW.GT.2) WRITE(101,1020 ) CON2 ,CC
      ICON = 0
      IF (CON2.LT.0.   ) GO TO 370
      CPAR = -CON2
      CON2 = CON2 * EPSLON
C
C       STEP TO THE LIMIT TO THE NEAREST CONSTRAINT TO CHECK FOR IMPROVEM
C
      DO 340 I=1,N
  340    PL(I) = XB(I) + NORM*P(I)
      FNUM = FNUM + 1
      CALL FVAL(PL,FL)
      IF (IW.GT.2) WRITE(101,1090 ) FNUM,FL, (PL(I),I=1,N)
      IF ((FB-FL).GE.NORM*CON2) GO TO 350
C
C
C       NO SIGNIFICANT IMPROVEMENT.  ATTEMPT TO LOCATE THE OPT. ALONG
C       THE DIRECTION P TO MORE DEFINITION.
C
C
      IF (IEXP.EQ.0) CALL CUBMIN(XB,FB,PL,FL,P,EXTRA,FVAL,N, CON2,NORM,
     > FNUM,IW,NLIN,LL,GRADNT,CC,CPAR)
      IF (IEXP.EQ.1) CALL PRBOLC(XB,FB,PL,FL,NORM,CON2,P,N,FNUM,FVAL,IW,
     > NLIN,LL, CC,FLOWER,ACC,CPAR)
      IF (FNUM.GT.FMAX) GO TO 740
      IF (LL.NE.2) GO TO 410
      GO TO 370
  350 DO 360 I=1,N
         EXT = PL(I) - XB(I)
         XB(I) = PL(I)
  360    PL(I) = EXT
      FB = FL
      ICON = 0
      IF (CC.LE.1.   ) ICON = 1
      GO TO 410
C
C       NO IMPROVEMENT IN THE FUNCTION.  SO RESET THE S MATRIX TO I.
C
  370 IF (IFRST.EQ.0) GO TO 750
      DO 390 I=1,N
         DO 380 K=1,N
  380       S(I,K) = 0.
  390    S(I,I) = 1.
      IFRST = 0
      IF (NBC.EQ.0) GO TO 670
C
C       RESET GTSG.
C
      LA = 0
      DO 400 I=1,NBC
         IC = COL(I)
  400    CALL CONADD(GTSG,S,IC,COL,P,PL,N,LA,IV,IC)
      GO TO 670
C
C
C       XB = X(K+1)      P = Q(K+1)       PL= P(K+1) THEN PL = P(K+1) - S(K
C
C       UPDATE S,GTSG FOR K+1  AND  POSSIBLY GTSG FOR NBC + 1.
C
  410 CALL GRADNT(XB,EXTRA)
      IF(IW.EQ.3)WRITE(101,1050)FNUM,FB,(XB(I),I=1,N)
      IF(IW.EQ.2)WRITE(101,1051)FNUM,FB,(XB(I),I=1,N)
      IF (FNUM.GT.FMAX) GO TO 740
      IFRST = 1
      DO 420 I=1,N
  420    P(I) = EXTRA(I) - PAR(I)
      DO 430 I=1,N
         IF ( ABS(P(I)).GT.TOL1) GO TO 440
  430    CONTINUE
      GO TO 370
  440 CONTINUE
C
C
C       RESCALE THE ALFA AND THE S MATRIX.  HOWEVER LEAVE THE STEP SIZE
C       UNALTERED.  THUS IF ALFA IS SCALED UP THE S IS SCALED DOWN.
C       ALSO SCALE THE S AND THE GTSG MATRIX TO SATISFY THE NORM RE-
C       QUIREMENT.
C
C
      CON2 = NORM
      AF = 1.
      IF (CON2.GE.DELTAP) GO TO 450
      AF = CON2/DELTAP
```

```
                                                    (NORM)
                                                    TO 450
                                                    TO 510
                                                    TO 510
                                                    NBC
                                                    GTSG(I,K)/AF
                                                    GO TO 510
                                                    NBC
                                                    GTSG(I,K)
```

```
1415            DO 640 J=1,LA
1416     640        GTSG(I,J) = GTSG(J,I)
1417     650 DO 660 I=1,N
1418     660    PAR(I) = EXTRA(I)
1419 C
1420 C
1421 C       GTSG HAS NOW BEEN ADJUSTED FOR S(K+1)
1422 C
1423 C
1424 C
1425 C
1426 C       NOW IF A CONSTRAINT HAS BEEN ADDED  ADD IT TO THE BASIS.
1427 C
1428     670 IF (ICON.EQ.0) GO TO 100
1429     680 IF (NBC.EQ.0) GO TO 690
1430         CALL PROJCT(PL,P,EXTRA,S,GTSG,N,NBC,COL,LL,IW,IC, NORM1)
1431         IF (IW.GT.2) WRITE(IO1,1120 ) LL,NORM1,TOL1
1432 C        TEST AGAINST TOL1 FOR LINEAR DEPENDENCE
1433         IF (NORM1.GT.TOL1) GO TO 690
1434         NDEP = NDEP + 1
1435         DEPC(NDEP) = LL
1436         GO TO 100
1437     690 CALL CONADD(GTSG,S,LL,COL,P,PL,N,NBC,IV,IC)
1438         IF (IW.GT.2) WRITE(IO1,1110 ) LL,NBC
1439         GO TO 100
1440     700 LL = 1
1441         GO TO 680
1442     710 CONTINUE
1443         IF((IW.GT.0).AND.(IW.NE.2))
1444        2            WRITE(IO1,1050 ) FNUM,FB,(XB(I),I=1,N)
1445         IF(IW.EQ.2)WRITE(IO1,1131)((LABEL1,LABEL2),I=1,LBLMAX)
1446         IF (IW.LT.1.OR.NBC.EQ.0) GO TO 760
1447         WRITE(IO1,1030 )
1448         WRITE(IO1,1140 )
1449         DO 720 I=1,NBC
1450            IO = COL(I)
1451     720    WRITE(IO1,1160 ) IO,(G(K,IO),K=1,N)
1452         IF (NDEP.EQ.0) GO TO 760
1453         WRITE(IO1,1030 )
1454         WRITE(IO1,1150 )
1455         WRITE(IO1,1140 )
1456         DO 730 I=1,NDEP
1457            IO = DEPC(I)
1458     730    WRITE(IO1,1160 ) IO,(G(K,IO),K=1,N)
1459         GO TO 760
1460     740 IF (IW.GT.0) WRITE(IO1,1180 ) FNUM,FMAX
1461         IFAIL = 1
1462         GO TO 760
1463     750 IF (IW.GT.0) WRITE(IO1,1190 )
1464         IFAIL = 2
1465     760 CONTINUE
1466         IF(NSEARCH.GT.0) GO TO 771
1467         DO 761 I=1,N
1468     761    XINF(I) = XB(I)
1469         FINF = FB
1470         GO TO 799
1471     771 IF(FB.GE.FINF) GO TO 2
1472         DO 772 I=1,N
1473     772    XINF(I) = XB(I)
1474         FINF = FB
1475         IFAILA = IFAIL
1476         GO TO 2
1477     798 IFAIL = IFAILA
1478         IF(IW.GT.0)WRITE(IO1,1052)NSEARCH,FINF,(XINF(I),I=1,N)
1479     799 RETURN
1480    1000 FORMAT(1H ,I10,2E20.10)
1481    1010 FORMAT(1H ,*NORM = *,E16.8,*   BETA =  *,E16.8, *  J =  *,I5////)
1482    1020 FORMAT(1H ,*INDEX OF IMPROVEMENT*,E18.8, 10X,
1483       1 *THE UPPER BOUND ON STEP SIZE*,E18.8/)
1484    1030 FORMAT(1H ,///)
1485    1040 FORMAT(1H ,3X,*N*,9X,*M*,8X,*NE*,6X,*IEXP*,6X,*ML1N*,6X,*FMAX*,
1486       1 8X,*IW*,/1H ,7110/1HO,4X,*CONVG*,6X,*DELT*,4X,*EPSLON*,6X,*RHO*
1487       2 ,4X,*DELTAP*,7X,*TOL1*/1H ,6E10.3//)
1488    1048 FORMAT(/,* ITERATION NO. *,I3,/,
1489       2 * FNUM    FUNCTION VALUE              Z(1)...*,/)
1490    1049 FORMAT(41H FNUM    FUNCTION VALUE              Z(1)...,/)
1491    1050 FORMAT(1H ,*THE NUMBER OF CALLS TO FVAL IS  *,I3/2H  , 7E16.8/ (
1492       1 2H   ,16X,6E16.8))
1493    1051 FORMAT(15,1X,7E16.8,/,(22X,6E15.8))
1494    1052 FORMAT(//,* BEST LOCAL MINIMUM FOUND AFTER *,I3,* TRYS IS...*,//,
1495       2 6X,7E16.8,/,(22X,6E16.8))
1496    1060 FORMAT(1H ,*THE CONSTRAINT* ,I3,*HAS BEEN PUT IN THE BASIS*,
1497       1 1H ,*THERE ARE*,I5,*CONSTRAINTS IN THE BASIS NOW.*)
1498    1070 FORMAT(1H ,  *THE COEFFICIENTS OF  THE NEW CONSTRAINT ARE*/ 1H ,
1499       1 7E16.8/(1H ,7E16.8))
1500    1080 FORMAT(1HO,*CONSTRAINT*,I5,  *  HAS BEEN DROPPED FROM THE BASIS*//)
1501    1090 FORMAT(1H ,*AFTER * ,I5,* CALLS THE MAXIMUM STEP TOWARD THE NEAREST
1502       1 CONSTRAINT GIVES*/1H ,7E16.8/1H ,16X,7E16.8))
1503    1100 FORMAT(1H ,*XXXX  RESET S FOR THE POSITIVE DEFINITE FAILURE*)
1504    1110 FORMAT(1H ,*THE CONSTRAINT  *,I5,  *  HAS BEEN PUT IN THE BASIS.*/
```

```
1505          1 1H ,*THERE ARE *,I5,* CONSTRAINTS IN THE PRESENT BASIS.*)
1506     1120 FORMAT(1HO,*THE PROJECTION OF CONSTRAINT *,I3,
1507          1 * AGAINST THE CURRENT BASIS IS *,E16.8,
1508          1 * THE TOLERANCE FOR LIN-DEP IS *,E16.8)
1509     1130 FORMAT(1H ,*AFTER  *,I5,*  CALLS THE CONVERGED POINT IS*/ 1H ,
1510          1 7E16.8/(1H ,16X,6E16.8))
1511     1131 FORMAT(6H ***,2(A6,A10))
1512     1140 FORMAT(1H ,*CONSTRAINT *,I0X,*COEFFICIENTS*//)
1513     1150 FORMAT(1HO,
1514          1 *THESE CONSTRAINTS ARE DEPENDENT ON THOSE IN THE BASIS *//)
1515     1160 FORMAT(1H ,I5,5X,6E16.8/(1H ,10X,6E16.8))
1516     1170 FORMAT(1HO,*THE S MATRIX MUST BE SCALED TO SATISFY NORMS.  THE *,,
1517          1 1H ,*NORM SCALE FACTOR IS *,E16.8)
1518     1180 FORMAT(1H ,*TOO MANY CALLS  *,2I10)
1519     1190 FORMAT(1H ,*THE IDENITY RESET USED IN SUCCESION*)
1520          END


1521          SUBROUTINE CONDRP(COL,J,NBC,GTSG,PL,IC)
1522          DIMENSION GTSG(IC,IC),PL(IC)
1523          INTEGER COL(IC)
1524          IF (J.EQ.NBC) GO TO 30
1525     C
1526     CC    SWITCH COLUMNS J,NBC           SWITCH ROWS J,NBC.
1527     C
1528          DO 10 I=1,NBC
1529          CC = GTSG(I,NBC)
1530             GTSG(I,NBC) = GTSG(I,J)
1531       10    GTSG(I,J) = CC
1532          DO 20 I=1,NBC
1533             CC = GTSG(NBC,I)
1534             GTSG(NBC,I) = GTSG(J,I)
1535       20    GTSG(J,I) = CC
1536     C
1537     CC       CALCULATE THE NEW INVERSE.
1538     C
1539       30 CONTINUE
1540          IF (NBC.GT.1) GO TO 40
1541          NBC = 0
1542          COL(1) = 0
1543          RETURN
1544       40 NB1 = NBC - 1
1545          CC = GTSG(NBC,NBC)
1546          DO 50 I=1,NB1
1547             CON1 = GTSG(I,NBC)
1548             DO 50 K=1,NB1
1549       50       GTSG(I,K) = GTSG(I,K) - CON1*GTSG(NBC,K)/CC
1550          IF (NB1.EQ.1) GO TO 70
1551          DO 60 I=2,NB1
1552             LA = I-1
1553             DO 60 K=1,LA
1554       60       GTSG(I,K)=GTSG(K,I)
1555       70 IF (J.LT.NB1) GO TO 80
1556          IF (J.EQ.NB1) COL(NB1) = COL(NBC)
1557          COL(NBC) = 0
1558          NBC = NB1
1559          RETURN
1560     C
1561     CC       ADJUST THE NEW MATRIX FOR J NE NBC BY SLIDING THE ROWS AND COLS.
1562     CC       BACK TO THE J-TH. AND PUTTING THE J-TH IN THE LAST.
1563     C
1564       80 DO 90 I=1,NB1
1565       90    PL(I) = GTSG(I,J)
1566          NB2 = NB1 - 1
1567          DO 100 K=J,NB2
1568             LA = K+1
1569             DO 100 I=1,NB1
1570      100       GTSG(I,K) = GTSG(I,LA)
1571          DO 110 I=1,NB1
1572      110 GTSG(I,NB1) = PL(I)
1573          DO 120 I=1,NB1
1574      120    PL(I) = GTSG(J,I)
1575          DO 130 K=J,NB2
1576             LA = K+1
1577             DO 130 I=1,NB1
1578      130       GTSG(K,I) = GTSG(LA,I)
1579          DO 140 I=1,NB1
1580      140    GTSG(NB1,I) = PL(I)
1581          DO 150 I=J,NB1
1582      150    COL(I) = COL(I+1)
1583          COL(NBC) = 0
1584          NBC = NB1
1585          RETURN
1586          END


1587          SUBROUTINE PROJCT(PL,P,EXTRA,S,GTSG,N,NBC,COL,I,IV,IC, NORM1)
1588     C
1589          DIMENSION P(1),PL(1),GTSG(IC,IC),S(IV,IV),EXTRA(1)
1590          REAL NORM1
```

```
      INTEGER COL(10),COLI,COLJ
      COMMON /S/S(20,20),N
C
C     THIS ROUTINE COMPUTES THE NORM OF THE PROJECTION OF THE I-TH
C     CONSTRAINT.
C
      DO 10 K=1,N
         EXTRA(K) = 0.
         DO 10 J=1,N
10       EXTRA(K) = EXTRA(K) + S(K,J)*G(J,I)
      DO 20 K=1,NBC
         PL(K) = 0.
         LA = COL(K)
         DO 20 J=1,N
20       PL(K) = PL(K) + G(J,LA)*EXTRA(J)
      DO 30 K=1,NBC
         P(K) = 0.
         DO 30 J=1,NBC
30       P(K) = P(K) + GTSG(K,J)*PL(J)
      DO 40 K=1,N
         PL(K) = 0.
         DO 40 J=1,NBC
            COLJ = COL(J)
40       PL(K) = PL(K) + G(K,COLJ)*P(J)
      DO 50 K=1,N
         P(K) = EXTRA(K)
         DO 50 J=1,N
50       P(K) = P(K) - S(K,J)*PL(J)
C
C     P IS NOW THE PROJECTION OF THE I-TH CONSTRAINT.
C
      NORM1 = 0.
      DO 60 K=1,N
60       NORM1 = NORM1 + P(K)**2
      NORM = SQRT(NORM1)
      RETURN
      END

      SUBROUTINE CONADD(GTSG,S,LL,COL,P,PL,N,NBC,IV,IC)
      DIMENSION GTSG(IC,IC),S(IV,IV),P(1),PL(1)
      INTEGER COL(IC),COLI,COLJ
      COMMON /DATA/W,H/ G(10,20),B(20)
C
C
C     THIS ROUTINE UPDATES THE MATRIX  (G(M)  - T * S(K) * G(M) )-INVER
C     TO THE MATRIX (G(M+1)-T * S(K) * G(M+1) ) - INVERSE WHEN THE LL
C     CONSTRAINT IS PUT IN THE BASIS.
C
C
C
      NP1 = NBC + 1
      COL(NP1) = LL
C
C     SET UP A12
C
      DO 10 I=1,N
         P(I) = 0.
         DO 10 J=1,N
10       P(I) = P(I) + S(I,J) * G(J,LL)
      A0 = 0.
      DO 30 I=1,N
20       A0 = A0 + G(I,LL) * P(I)
      IF (NBC.EQ.0) GO TO 100
      DO 30 I=1,NBC
         PL(I) = 0.
         DO 30 J=1,N
            COLI = COL(I)
30          PL(I) = PL(I) + G(J,COLI) * P(J)
C
C
C     SET UP -A11-1  *  A12
C
C
      DO 40 I=1,NBC
         P(I) = 0.
         DO 40 J=1,NBC
40          P(I) = P(I) - GTSG(I,J) * PL(J)
C
C     COMPLETE CALCULATION OF A0
C
      DO 50 I=1,NBC
50       A0 = A0 + PL(I) * P(I)
      DO 60 I=1,NBC
         DO 60 J=1,NBC
60       GTSG(I,J) = GTSG(I,J) + P(I) * P(J) / A0
      IF (NBC.EQ.1) GO TO 80
      DO 70 I=2,NBC
         LA = I-1
         DO 70 J=1,LA
70          GTSG(I,J) = GTSG(J,I)
```

```
      80 DO 90 I=1,NBC
         GTSG(I,NB1) = P(I)/AO
      90 GTSG(NB1,I) = GTSG(I,NB1)
     100 GTSG(NB1,NB1) = 1./AD
         NBC = NB1
         RETURN
         END


         SUBROUTINE CUBMIN(XB,FB,PL,FL,P,EXTRA,FVAL,N,CON2, DST ,FNUM,IW,
        1 NLIN,LL,GRADNT,CC,CPAR)
C
         DIMENSION XB(1),P(1),PL(1),EXTRA(1)
         REAL NORM,NORM1
         INTEGER FNUM
C        IO1 IS THE LOGICAL UNIT NUMBER FOR PRINTOUT
         IO1 = 3
         LL = 0
         NL = 0
         NORM = DST
         CALL GRADNT(PL,EXTRA)
         GB = 0.
         DO 10 I=1,N
      10    GB = GB + P(I) * EXTRA(I)
         GA = CPAR
         IF (GB.GT.0.   ) GO TO 120
         GO TO 30
      20 LL = 2
         FNUM = FNUM + NL
         RETURN
      30 IF (CC.GT.NORM) GO TO 80
      40 NORM = NORM / 2.
         DO 50 I=1,N
      50    PL(I) = XB(I) + NORM * P(I)
         NL = NL + 1
         CALL FVAL( PL ,FE)
         IF (IW.GT.2) WRITE(IO1,1000 ) FE, NORM
         IF ((FB-FE).GE.NORM*CON2) GO TO 60
         IF (NL.LE.NLIN) GO TO 40
         GO TO 20
      60 CALL GRADNT(PL,EXTRA)
         GB = 0.
         DO 70 I=1,N
      70    GB = GB + P(I)*EXTRA(I)
         IF (GB.LE.0.   ) GO TO 210
         FL = FE
         GO TO 120
      80 GA = GB
         F1 = FL
         NORM1 = NORM
C        NORM = DMIN1(NORM1 + DST,CC)
         NORM = NORM1 + DST
         IF(NORM.GT.CC) NORM = CC
         DO 90 I=1,N
      90    PL(I) = XB(I) + NORM*P(I)
         CALL GRADNT(PL,EXTRA)
         GB = 0.
         DO 100 I=1,N
     100    GB = GB + P(I) * EXTRA(I)
         CALL FVAL(PL,FL)
         IF (IW.GT.2) WRITE(IO1,1020 ) FL, NORM
         NL = NL + 1
         IF (GB.GT.0.   ) GO TO 110
         IF ((FB-FL).GE.NORM*CON2) GO TO 200
         IF (NORM.GE.CC) GO TO 20
         IF (NL.LT.NLIN) GO TO 80
         GO TO 20
     110 A = NORM1
         B = NORM
         GO TO 140
     120 A = 0.
         B = NORM
         F1 = FB
         GO TO 140
     130 IF (NL.GT.NLIN) GO TO 20
     140 Z = 3. *((F1-FL)/(B-A))+GA+GB
         W = SQRT(Z*Z-GA*GB)
         AS = B - ((GB+W-Z)/(GB-GA+2.00*W)) * (B-A)
         IF (A.LT.AS.AND.AS.LT.B) GO TO 150
         AS = .5*(A+B)
     150 DO 160 I=1,N
     160    PL(I) = XB(I) + AS * P(I)
         NL = NL + 1
         CALL FVAL(PL,FE)
         IF (IW.GT.2) WRITE(IO1,1010 ) FE,AS
         IF ((FE-FB).GE.AS*CON2) GO TO 170
         NORM = AS
         GO TO 210
     170 CALL GRADNT(PL,EXTRA)
         Z = 0.
```

```
      DO 180 I=1,N
  180    Z = Z + P(I)*EXTRA(I)
      IF (Z.GE.0.   ) GO TO 190
      A = AS
      GA = Z
      F1 = FE
      GO TO 130
  190 B = AS
      FL = FE
      GB = Z
      GO TO 130
  200 FE = FL
  210 DO 220 I=1,N
      W = PL(I) - XB(I)
      XB(I) = PL(I)
  220    PL(I) = W
      FB = FE
      FNUM = FNUM + NL
      DST = NORM
      RETURN
 1000 FORMAT(3H H , E20.12,5X,E15.6)
 1010 FORMAT(3H C , E20.12,5X,E15.6)
 1020 FORMAT(3H E , E20.12,5X,E15.6)
      END

      SUBROUTINE PRBOLC(XB,FB,PL,FL,DST,CON2,P,N,FNUM,FVAL,IW,LINMIN,
     > LL,CC,FLOWER,ACC,CPAR)
      REAL NORM
      REAL L1,L2,L3
      DIMENSION XB(1),P(1),PL(1)
      INTEGER FNUM
C     IO1 IS THE LOGICAL UNIT NUMBER FOR PRINTOUT
      IO1 = 3
      IF (FB.LT.FLOWER) FLOWER = -1.E+30
      IWK = 0
      LL = 0
      NLN = 0
      NORM = CPAR
      CON = -NORM
      NORM = 2.   * ABS((FB-FLOWER)/NORM)
C     RO = DMIN1(NORM,1.D0,.5D0*CC)
      RO = .5*CC
      IF(RO.GT.1.) RO = 1.
      IF(RO.GT.NORM) RO = NORM
      IF (RO.EQ.DST) GO TO 20
      DO 10 I=1,N
   10    PL(I) = XB(I) + RO*P(I)
      CALL FVAL(PL,F1)
      IF (IW.GT.2) WRITE(IO1,1010 ) F1,RO
      NLN = NLN + 1
      IF (NLN.GE.LINMIN) GO TO 240
      GO TO 30
   20 F1 = FL
   30 LO = 0.
      L1 = RO
      FO = FB
   40 R1 = .5   *CON*RO*RO/(F1-FO+ CON*RO)
      IF (R1.GT.O.   ) GO TO 60
C  50 L2 = DMIN1(2.D0*L1,L1 + .999*(CC-L1))
   50 L2 = L1 + .999*(CC-L1)
      IF(L2.GT.(2.*L1)) L2 = 2.*L1
   60 DO 70 I=1,N
   70    PL(I) = XB(I) + L2*P(I)
      CALL FVAL(PL,F2)
      IF (IW.GT.2) WRITE(IO1,1010 ) F2,L2
      NLN = NLN + 1
      IF (NLN.GT.LINMIN) GO TO 230
      IF (F2.GE.F1) GO TO 140
      LO = L1
      FO = F1
      L1 = L2
      F1 = F2
      GO TO 50
   80 IF (R1-L1) 100,50,90
C  90 L2 = DMIN1(R1,.999*CC)
   90 L2 = .999*CC
      IF(L2.GT.R1) L2 = R1
      GO TO 60
C 100 D = DMIN1(.75D0*RO,R1)
  100 D = .75*RO
      IF(D.GT.R1) D = R1
C     R2 = DMAX1(.25D0*RO,D)
      R2 = .25*RO
      IF(R2.LT.D) R2 = D
      DO 110 I=1,N
  110    PL(I) = XB(I) + R2*P(I)
      CALL FVAL(PL,NORM)
      IF (IW.GT.2) WRITE(IO1,1010 ) NORM,R2
      NLN = NLN + 1
```

```
      IF (NLN.GT.LINMIN) GO TO 240
      IF (NORM.LT.F0) GO TO 120
      L1 = R2
      F1 = NORM
      R0 = R2
      GO TO 40
  120 IF (NORM.LE.F1) GO TO 130
      L0 = R2
      F0 = NORM
      GO TO 50
  130 L2 = L1
      F2 = F1
      L1 = R2
      F1 = NORM
  140 K = 1
      IF (IWK.EQ.0) GO TO 150
      IF ((FB-F1).GE.L1*CON2) GO TO 260
  150 IWK = 1
      R3 = .500*(F0*(L1**2-L2**2) + F1*(L2**2-L0**2) + F2*( L0**2-L1**2:
     > )/(F0*(L1-L2) + F1*(L2-L0) + F2*(L0-L1))
      IF ( ABS(R3-L1).LE.ACC*L1) GO TO 260
C     D = DMIN1(L0+.9D0*(L2-L0),R3)
      D = L0 + .9*(L2-L0)
      IF(D.GT.R3) D = R3
C     R4 = DMAX1(L0+.1D0*(L2-L0),D)
      R4 = L0 + .1*(L2-L0)
      IF(R4.LT.D) R4 = D
  160 DO 170 I=1,N
  170    PL(I) = XB(I) + R4*P(I)
      CALL FVAL(PL,NORM)
      IF (IW.GT.2) WRITE(101,1000 ) NORM,R4
      NLN = NLN + 1
      IF (NLN.GT.LINMIN) GO TO 240
      IF (R4.EQ.L1) GO TO 260
      IF (R4.GT.L1) GO TO 210
      IF (NORM.LT.F1) GO TO 190
      L0 = R4
      F0 = NORM
      IF (K.EQ.2) GO TO 140
      R4 = .5*(L1+L2)
  180 K = 2
      GO TO 160
  190 L2 = L1
      F2 = F
  200 L1 = R
      F1 = NORM
      GO TO 140
  210 IF (NORM.GE.F1) GO TO 220
      L0 = L1
      F0 = F1
      GO TO 200
  220 L2 = R4
      F2 = NORM
      IF (K.EQ.2) GO TO 140
      R4 = .5*(L1+L2)
      GO TO 180
  230 IF (F2.GE.F1) GO TO 240
      F1 = F2
      L1 = L2
  240 LL = 2
      IF (((FB-F1).LT.CON2*L1) GO TO 280
      LL = 1
      DO 250 I=1,N
  250    PL(I) = XB(I) + L1*P(I)
  260 IF (FB.LE.F1) GO TO 240
      FB = F1
      OST = L1
      DO 270 I=1,N
         D = PL(I) - XB(I)
         XB(I) = PL(I)
  270    PL(I) = D
  280 FNUM = FNUM + NLN
      RETURN
 1000 FORMAT(3H0B ,E25.12,5X,E15.6)
 1010 FORMAT(3H0S ,E25.12,5X,E15.6)
      END


      SUBROUTINE PAYNTER (K,KMAX,N1,DELTA,ERROR,NOUT,A,NO)
C     THIS ROUTINE HAS OUTPUT TO UNIT (NOUT).
C
C THIS SUBROUTINE SOLVES FOR THE PAYNTER TRUNCATION NUMBER K. SOLVE FOR
C A K SUFFICIENTLY LARGE THAT THE FOLLOWING INEQUALITY IS SATISFIED:
C        (1/FACTORIAL(K))*(Q**K)*EXP(Q)<ERROR
C
C     REF.  ANALYSIS,SIMULATION, AND CONTROL OF DYNAMIC SYSTEMS BY J. W
C     BREWER PP180-182 FOR THE JUSTIFICATION OF THIS METHOD.
C     AND, MCCUE, H. K., UNIVERSITY OF CALIFORNIA,
C     LAWRENCE LIVERMORE LABORATORY (PRIVATE COMMUNICATION).
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C THE LARGEST FACTORIALS THAT ONE CAN REPRESENT ON A 60 BIT MACHINE
C ARE AS FOLLOWS:
C                 18 FACTORIAL                    INTEGER
C                 164 FACTORIAL                   FLOATING POINT
C THIS FACT ALONG WITH HOW ONE IMPLIMENTS THE PAYNTER INEQUALITY
C PLACES AN UPPER BOUND ON KMAX (ASSUMING SINGLE PRECISION).
C A REASONABLE VALUE IS KMAX=100 FOR FLOATING POINT FACTORIALS.
C
      DIMENSION A(ND,ND)
C
C SET K=0 FOR CHECK ON RETURN.
      K=0
C SOLVE FOR THE LARGEST ELEMENT IN THE A MATRIX.
      AMAX = ABS(A(1,1))
      DO 1 I=1,N1
      DO 1 J=1,N1
      Q=ABS(A(I,J))
1     IF(Q.GT.AMAX)AMAX=Q
C SCALE AMAX TO THE REQUIRED VALUE.
      Q=AMAX*DELTA**N
C
C PERFORM THE PAYNTER INEQUALITY AND SOLVE FOR K.
      AMAX=EXP(Q)
      X1=0.0
      XK=0.0
      DO 2 I=1,KMAX
      XK=XK+1.0
      X1=Q/XK
      AMAX=AMAX*X1
      IF(AMAX.LE.1.0)GO TO 10
2     CONTINUE
C INEQUALITY WAS NOT SATISFIED FOR K=KMAX.
      K = -1
      GO TO 11
C THE INEQUALITY WAS SATISFIED FOR K=I.
10    K=I
11    CONTINUE
      WRITE (6,101) K,KMAX,DELTA
101   FORMAT (/ 'K = ',I5,' KMAX = ',I5,' DELTA = ',F10.3,
     2 /' K = -1 IMPLIES DELTA = 1.0 E-7.'
     3 /' EITHER THE MATRIX IS NOT POSITIVE DEFINITE OR KMAX IS TOO SMALL.'
     4 /' SEE THE COMMENTS IN THE SUBROUTINE FOR MORE DETAILS.')
999   CONTINUE
      RETURN
      END


      SUBROUTINE SIMUL(N,D,A,B,X,SAPW,T,Q,R,WKRT,KS,DET,A,ND)
C     THIS PROGRAM FINDS THE SOLUTION
C
C     SPECIAL CASE...A(I,J) IS DIAGONAL
C
C     THIS SUBROUTINE IS USED TO FIND THE STEADY STATE COVARIANCE
C     NOISE TRANSITION MATRIX FOR A SAMPLED DATA SYSTEM
C     X(K) = D*X(K-1) + W(K-1)  E(K,K-1)=D*E(K-1)*D(T) + Q
C     GIVEN THE MATRIX D AND Q FOR THE DISCRETE SYSTEM
C       X(T)DOT = A*X(T) + B*U(T) + D*W(T).
C
C      P=SUMMATION I=1 TO N OF(A(I,I)**I)*Q*(A(I,I)**I) FACTORIAL))
C      Q=SUMMATION I=1 TO N OF (A**I)*B*B*(A**I)/(I FACTORIAL)
C      R=SUMMATION I=1 TO N OF (A**I)*B*(A**(I+1) FACTORIAL)
C
C     IT ALSO COMPUTES THE STATE NOISE COVARIANCE MATRIX SAPW
C     WHERE,
C      FTLD(I) = (1/I)*(ATLD(I-1)*DTLD - DTLD(I)*(A(T)), FTLD(0) = 0,
C      ATLD(I) = (AT/I)*(ATLD(I-1), ATLD(0) = I
C      PHI21 = SUMMATION I=1 TO N OF FTLD(I),
C      PHI22 = SUMMATION I=0 TO N-1 OF ATLD(I), AND FINALLY,
C      WKRT(TK,TK-1) = PHI21 * (PHI22)**T
C
C     REF...D'APPOLITO, J. A., A SIMPLE ALGORITHM FOR DISCRETIZING
C     LINEAR STATIONARY CONTINUOUS SYSTEMS, IEEE TRANS. ON AUTO. CONT., VOL. 14, NO. 12,
C     PP. 2010,2011, DEC. 1968, AND
C     GELB, A.(ED.), APPLIED OPTIMAL ESTIMATION, MIT PRESS, 1974, OR
C     COURSE NOTES, A SHORT COURSE ON LINEAR FILTERING AND APPLICATIONS
C     THE ANALYTIC SCIENCES CORPORATION, READING, MASSACHUSETTS, 1969
C
      DIMENSION A(10,10),B(10,10),D(10,10),P(10,10),Q(10,10),R(10,10)
      DIMENSION S(10),SUM(10),ATLD(10,10),SAPW(10,10),WKRT(10,10)
     2 PHI21(10,10),PHI22(10,10),FTLD(10,10),ATLD(10,10),DTLD(10,10)
      ND = 10
C INITIALIZE THE MATRICES.
      CALL ADDTBT (SAPW,D,FTLD,N3,N3,N1,ND)
      CALL ADDTB  (D,FTLD,DTLD,N1,N3,N1,ND)
      DO 2 I=1,N1
      DO 1 J=1,N1
      DTLD(I,J) = DTLD(I,J)*DELTA
      P(I,J) = 0.
      PHI21(I,J) = 0.
1     FTLD(I,J) = 0.
```

```
      AT(I) = A(I,I)*DELTA
      SUM(I) = 1.
      S(I) = 1.
      PHI22(I) = 1.
2    ATLD(I) = 1.
C     COMPUTE STATE NOISE COVARIANCE TRANSITION MATRIX WKP1(TK,TK-1)
C     AND STATE TRANSITION MATRIX P(TK,TK-1)...
      KKM1 = KK-1
      DO 5 K=1,KKM1
      DO 4 I=1,N1
      DO 3 J=1,N1
      FTLD(I,J) = (ATLD(I)*DTLD(I,J) - FTLD(I,J)*AT(J))/K
3     PHI21(I,J) = PHI21(I,J) + FTLD(I,J)
      ATLD(I) = AT(I)*ATLD(I)/K
4     PHI22(I) = PHI22(I) + ATLD(I)
5     CONTINUE
      DO 7 I=1,N1
      DO 6 J=1,N1
C     NOTE...SINCE A IS DIAGONAL, PHI22 = (PHI22)T
6     WKP1(I,J) = PHI21(I,J)*PHI22(J)
7     P(I,I) = PHI22(I)
C     COMPUTE (SUM), THE INTERMEDIATE SUMMATION TIMES (DELTA)...
      DO 15 J=2,KK
      DO 14 I=1,N1
      S(I) = S(I) * AT(I)/J
14    SUM(I) = SUM(I) + S(I)
15    CONTINUE
      IF(N2.EQ.0) GO TO 10
C     COMPUTE CONTROL TRANSITION MATRIX Q(TK,TK-1)...
      DO 18 I=1,N1
      DO 17 J=1,N2
17    Q(I,J) = DELTA*SUM(I)*B(I,J)
18    CONTINUE
10    CONTINUE
C     COMPUTE NOISE TRANSITION MATRIX R(TK,TK-1)...
      DO 20 I=1,N1
      DO 19 J=1,N3
19    R(I,J) = DELTA*SUM(I)*D(I,J)
20    CONTINUE
      CALL MATOUTP (P,N1,N1,2HAK,ND)
      IF(N2.NE.0) CALL MATOUTP (Q,N1,N2,2HBK,ND)
      CALL MATOUTP (R,N1,N3,2HDK,ND)
      CALL MATOUTP (WKP1,N1,N1,4HWKP1,ND)
      RETURN
      END


      SUBROUTINE ATOB  (A,B,N,M,ND)
C     COPIES (A) INTO (B)...
      DIMENSION A(10,10),B(10,10)
      DO 2 I=1,N
      DO 1 J=1,M
1     B(I,J) = A(I,J)
2     CONTINUE
      RETURN
      END


      SUBROUTINE ADOTB  (A,B,C,L,M,N,ND)
C     ROUTINE PERFORMS FOLLOWING MATRIX MULTIPLICATION...
C     C(LXN)  =  A(LXM) . B(MXN)
      DIMENSION A(10,10),B(10,10),C(10,10)
      DO 30 I = 1,L
      DO 20 J = 1,N
      C(I,J) = 0.0
      DO 10 K = 1,M
10    C(I,J) = C(I,J) + A(I,K)*B(K,J)
20    CONTINUE
30    CONTINUE
      RETURN
      END


      SUBROUTINE ADOTBT (A,B,C,L,M,N,ND)
C     ROUTINE PERFORMS FOLLOWING MATRIX MULTIPLICATION...
C     C(LXN)  =  A(LXM) . BT(MXN)
C     DIMENSIONS (L,M,N) REFER TO MATRICES AFTER THEY ARE TRANSPOSED.
      DIMENSION A(10,10),B(10,10),C(10,10)
      DO 30 I = 1,L
      DO 20 J = 1,N
      C(I,J) = 0.0
      DO 10 K = 1,M
10    C(I,J) = C(I,J) + A(I,K)*B(J,K)
20    CONTINUE
30    CONTINUE
      RETURN
      END


      SUBROUTINE ATOBTB (A,B,C,L,M,N,ND)
```

```
      C     ROUTINE PERFORMS FOLLOWING MATRIX MULTIPLICATION...
      C     C(LXN)  =  AT(LXM)  B(MXN)
      C     DIMENSIONS (L,M,N) REFER TO MATRICES AFTER THEY ARE TRANSPOSED.
            DIMENSION A(10,10),B(10,10),C(10,10)
            DO 30 I = 1,L
            DO 20 J = 1,N
            C(I,J) = 0.0
            DO 10 K = 1,M
        10  C(I,J) = C(I,J) + A(K,I)*B(K,J)
        20  CONTINUE
        30  CONTINUE
            RETURN
            END

            SUBROUTINE APLUSB (A,B,C,N,M,ND)
            DIMENSION A(10,10),B(10,10),C(10,10)
            DO 2 I = 1,N
            DO 1 J = 1,M
        1   C(I,J) = A(I,J) + B(I,J)
        2   CONTINUE
            RETURN
            END

            SUBROUTINE AMINSB (A,B,C,N,M,ND)
            DIMENSION A(10,10),B(10,10),C(10,10)
            DO 2 I = 1,N
            DO 1 J = 1,M
        1   C(I,J) = A(I,J) - B(I,J)
        2   CONTINUE
            RETURN
            END

            SUBROUTINE APLUSBT (A,B,C,N,M,ND)
            DIMENSION A(10,10),B(10,10),C(10,10)
      C     PERFORMS FOLLOWING MATRIX OPERATION
      C     C(NXM) = A(NXM) + BT(NXM)
            DO 2 I=1,N
            DO 1 J=1,M
        1   C(I,J) = A(I,J) + B(J,I)
        2   CONTINUE
            RETURN
            END

            SUBROUTINE ABAT (A,B,C,N,ND)
      C     COMPUTES C = A*B*AT FOR SPECIAL CASE WHERE (B) IS DIAGONAL...
            DIMENSION A(10,10),B(10,10),C(10,10)
            DO 2 I=1,N
            DO 1 J=1,N
        1   C(I,J) = A(I,I)*B(I,J)*A(J,J)
        2   CONTINUE
            RETURN
            END

            FUNCTION TR(A,N)
            DIMENSION A(10,10)
            TR = 0.
            DO 1 I=1,N
        1   TR = TR + A(I,I)
            RETURN
            END

            SUBROUTINE XTAY (X,A,Y,Q,N,ND)
      C     FINDS VALUE OF QUADRATIC FORM Q = XT*A*Y...
            DIMENSION X(10),A(10,10),Y(10)
            Q = 0.
            DO 2 J=1,N
            XA = 0.
            DO 1 I=1,N
        1   XA = XA + X(I)*A(I,J)
        2   Q = Q + XA*Y(J)
            RETURN
            END

            SUBROUTINE INVERSE (NN,A,AINV,IERROR)
      C     VER VER 9/74 - FOR FIXED DIMENSIONS (ND = 10)
      C
      C     SUBROUTINE COMPUTES THE INVERSE IF AN NXN REAL MATRIX (A) AND
      C     RETURNS IT IN (AINV).  (A) IS NOT DISTURBED IN THE PROCESS.
      C     GAUSSIAN ELIMINATION USING THE LU DECOMPOSITION AND
      C     ITERATIVE IMPROVEMENT IS THE METHOD FOR SOLUTION.
      C
      C     REF...MCCUE, H. K., UNIVERSITY OF CALIFORNIA,
      C     LAWRENCE LIVERMORE LABORATORY (PRIVATE COMMUNICATION), AND
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C      REF: G.FORSYTHE & CLEVE B. MOLER, COMPUTER SOLUTION
C      OF LINEAR ALGEBRAIC SYSTEMS, PRENTICE-HALL(1967), CHAPT. 17.
C
C      ON RETURN, IERROR IS THE ERROR FLAG.  IT SHOULD BE CHECKED.
C      IERROR = 0, EVERYTHING SEEMED OK.
C      IERROR = -1, ROW WITH ALL ZERO ELEMENTS WAS FOUND.
C      IERROR = -2, ZERO PIVOT ELEMENT WAS FOUND.
C      IERROR = -3, ITERATIVE IMPROVEMENT DID NOT CONVERGE, THE A MATRIX
C      IS ILL-CONDITIONED SUCH THAT NO SIGNIFICANT DIGITS OF THE
C      TRUE SOLUTION WERE OBTAINED IN THE ORIGINAL SOLUTION FROM SOLVE.
C
C      NOTE...VARIABLE DIMENSIONING IS USED THROUGHOUT THIS PACKAGE.
C      ND = SIZE OF DIMENSIONED ARRAYS IN CALLING ROUTINE.
C      NN = THE ACTUAL PROBLEM SIZE BEING USED (NN.LE.ND, OF COURSE).
C
C
      DIMENSION A(10,10),AINV(10,10),UL(10,10),B(10),X(10),
     2          SCALES(10),R(10),DX(10),IPS(10)
      IF(NN.EQ.1)GO TO 10
      ND = 10
      CALL DECOMP (NN,A,UL,SCALES,IPS,IERROR,ND)
      IF (IERROR.LT.0) RETURN
      INDEX=1
      DO 1 I=1,NN
C GENERATE THE PROPER B VECTOR.
      DO 2 J=1,NN
      B(J)=0.0
 2    CONTINUE
C SOLVE FOR THE COLUMN OF INVERSE.
      B(INDEX)=1.0
      CALL SOLVE (NN,UL,B,X,IPS,ND)
      CALL IMPROV (NN,A,UL,B,X,R,DX,IPS,DIGITS,IERROR,ND)
      IF (IERROR.LT.0) RETURN
C STORE COLUMN IN INVERSE MATRIX.
      DO 3 J=1,NN
      AINV(J,INDEX) = X(J)
 3    CONTINUE
      INDEX=INDEX+1
 1    CONTINUE
      RETURN
C     SCALAR CASE
 10   CONTINUE
      IF(A)11,20,11
 11   AINV = 1./A
      IERROR = 0
      RETURN
 20   IERROR = -2
      RETURN
      END


      SUBROUTINE DECOMP (NN,A,UL,SCALES,IPS,IERROR,ND)
      DIMENSION A(ND,ND),UL(ND,ND),SCALES(ND),IPS(ND)
      N = NN
C
C     INITIALIZE IPS, UL AND SCALES
      DO 5 I = 1,N
         IPS(I) = I
         ROWNRM = 0.0
         DO 2 J = 1,N
            UL(I,J) = A(I,J)
            IF(ROWNRM-ABS(UL(I,J))) 1,2,2
 1          ROWNRM = ABS(UL(I,J))
 2       CONTINUE
      IF (ROWNRM) 3,91,3
 3    SCALES(I) = 1.0/ROWNRM
 5    CONTINUE
C
C     GAUSSIAN ELIMINATION WITH PARTIAL PIVOTING
      NM1 = N-1
      DO 17 K = 1,NM1
         BIG = 0.0
         DO 11 I = K,N
            IP = IPS(I)
            SIZE = ABS(UL(IP,K))*SCALES(IP)
            IF (SIZE-BIG) 11,11,10
 10            BIG = SIZE
               IDXPIV = I
 11      CONTINUE
      IF (BIG) 13,92,13
 13      IF (IDXPIV-K) 14,15,14
 14         J = IPS(K)
            IPS(K) = IPS(IDXPIV)
            IPS(IDXPIV) = J
 15      KP = IPS(K)
         PIVOT = UL(KP,K)
         KP1 = K+1
         DO 16 I = KP1,N
            IP = IPS(I)
            EM = -UL(IP,K)/PIVOT
```

```
2277                UL(IP,K) = -EM
2278                DO 16 J = KP1,N
2279                   UL(IP,J) = UL(IP,J) + EM*UL(KP,J)
2280 C              INNER LOOP.  USE MACHINE LANGUAGE CODING IF COMPILER
2281 C           DOES NOT PRODUCE EFFICIENT CODE.
2282       16    CONTINUE
2283       17 CONTINUE
2284          KP = IPS(N)
2285          IF(UL(KP,N)) 19,92,19
2286    19    IERROR = 0
2287          RETURN
2288 C        ERROR EXITS...
2289 C        IERROR =  0, EVERYTHING SEEMED OK.
2290 C        IERROR = -1, ROW WITH ALL ZERO ELEMENTS WAS FOUND.
2291 C        IERROR = -2, ZERO PIVOT ELEMENT WAS FOUND.
2292    91    IERROR = -1
2293          RETURN
2294    92    IERROR = -2
2295          RETURN
2296          END


2297          SUBROUTINE SOLVE (NN,UL,B,X,IPS,ND)
2298          DIMENSION UL(ND,ND),B(ND),X(ND),IPS(ND)
2299          N = NN
2300          NP1 = N+1
2301 C
2302          IP = IPS(1)
2303          X(1) = B(IP)
2304          DO 2 I = 2,N
2305             IP = IPS(I)
2306             IM1 = I-1
2307             SUM = 0.0
2308             DO 1 J = 1,IM1
2309       1        SUM = SUM + UL(IP,J)*X(J)
2310       2  X(I) = B(IP) - SUM
2311 C              .
2312          IP = IPS(N)
2313          X(N) = X(N)/UL(IP,N)
2314          DO 4 IBACK = 2,N
2315          I = NP1-IBACK
2316 C           I GOES (N-1),...,1
2317             IP = IPS(I)
2318             IP1 = I+1
2319             SUM = 0.0
2320             DO 3 J = IP1,N
2321       3        SUM = SUM + UL(IP,J)*X(J)
2322       4  X(I) = (X(I)-SUM)/UL(IP,I)
2323          RETURN
2324          END


2325          SUBROUTINE IMPRUV (NN,A,UL,B,X,R,DX,IPS,DIGITS,IERROR,ND)
2326          DIMENSION A(ND,ND),UL(ND,ND),B(ND),X(ND),R(ND),DX(ND),IPS(ND)
2327 C        USES ABS(), AMAX1(), ALOG10()
2328          DOUBLE PRECISION SUM
2329          N = NN
2330 C
2331 C        XXX  EPS AND ITMAX ARE MACHINE DEPENDENT.  XXX
2332          EPS = 2.**(-47)
2333          ITMAX = 20
2334 C
2335          XNORM = 0.0
2336          DO 1 I = 1,N
2337       1     XNORM = AMAX1(XNORM,ABS(X(I)))
2338          IF (XNORM) 3,2,3
2339       2     DIGITS = -ALOG10(EPS)
2340             GO TO 10
2341 C
2342       3  DO 9 ITER = 1,ITMAX
2343             DO 5 I = 1,N
2344                SUM = 0.0
2345                DO 4 J = 1,N
2346       4           SUM = SUM + A(I,J)*X(J)
2347             SUM = B(I) - SUM
2348       5     R(I) = SUM
2349 C           XXX IT IS ESSENTIAL THAT A(I,J)*X(J) YIELD A DOUBLE PRECISION
2350 C           RESULT AND THAT THE ABOVE + AND - BE DOUTLE PRECISION. XXX
2351             CALL SOLVE (N,UL,R,DX,IPS,ND)
2352             DXNORM = 0.0
2353             DO 6 I = 1,N
2354                T = X(I)
2355                X(I) = X(I) + DX(I)
2356                DXNORM = AMAX1(DXNORM,ABS(X(I)-T))
2357       6     CONTINUE
2358             IF (ITER-1) 8,7,8
2359       7        DIGITS = -ALOG10(AMAX1(DXNORM/XNORM,EPS))
2360       8     IF (DXNORM-EPS*XNORM) 10,10,9
2361       9  CONTINUE
2362 C        ERROR EXIT...
```

```
2363 C      IERROR =  0, OK.
2364 C      IERROR = -9, ITERATIVE IMPROVEMENT DID NOT CONVERGE, THE A MATRIX
2365 C      IS ILL-CONDITIONED SUCH THAT NO SIGNIFICANT DIGITS OF THE
2366 C      TRUE SOLUTION WERE OBTAINED IN THE ORIGINAL SOLUTION FROM SOLVE.
2367         IERROR = -9
2368         RETURN
2369   10    IERROR =  0
2370         RETURN
2371         END


2372         SUBROUTINE NOISE (XBAR,CAPX,X,N,ND)
2373         DIMENSION XBAR(ND), CAPX(ND,ND), X(ND)
2374 C       RETURNS A RANDOM VECTOR (X) WHOSE ELEMENTS X(I)
2375 C       ARE NORMALLY DISTRIBUTED ABOUT A MEAN VALUE VECTOR (XBAR)
2376 C       WITH A (DIAGONAL) COVARIANCE (CAPX).
2377 C       THAT IS,
2378 C            X ~ N (XBAR,CAPX).
2379 C       NOTE ... IT IS ASSUMED THAT CAPX IS A DIAGONAL MATRIX.
2380 C
2381         DO 10 I=1,N
2382   10    X(I) = GN(XBAR(I),CAPX(I,I))
2383         RETURN
2384         END


2385         SUBROUTINE NOISEW (T,CAPX,X,SIGMA,N,ND)
2386         DIMENSION CAPX(ND,ND), X(ND), SIGMA(ND)
2387         COMMON /IO/ NIN,NOUT,NTTY,NRUN,VER
2388         DATA NENTER /0/
2389 C       RETURNS A RANDOM VECTOR (X) WHOSE ELEMENTS X(I) HAVE VARIANCE
2390 C       CAPX(I,I), CAPX BEING THE COVARIANCE MATRIX FOR X, THAT IS,
2391 C       CAPX = E(X,XT).
2392 C       NOTE ... IT IS ASSUMED THAT CAPX IS A DIAGONAL MATRIX.
2393 C XXX   CAUTION XXX THIS ROUTINE HAS MEMORY..USE FOR ONLY ONE VARIABLE XX)
2394 C       THIS ROUTINE (NOISEW) USED FOR PLANT DISTURBANCE VECTOR (W).
2395 C       NOTE...BY REMOVING STMT 1 BELOW, THE ROUTINE WILL ACCOMODATE
2396 C       TIME-VARYING STATISTICS (IE, CAPX(T).NE.CONST, ETC.)
2397    1    IF (NENTER.EQ.NRUN) GO TO 5
2398         NENTER = NRUN
2399 C       THIS FORM FOR TIME INVARIANT STATISTICS SUCH THAT STANDARD
2400 C       DEVIATIONS ARE CALCULATED ONLY AT BEGINNING OF RUN.
2401 C       GENERAL CASE WOULD BE TO CALCULATE SIGMA(T) A FUNCTION OF TIME.
2402 C       DETERMINE STANDARD DEVIATIONS FIRST TIME THROUGH
2403         DO 2 I=1,N
2404    2    SIGMA(I) = SQRT(CAPX(I,I))
2405    5    DO 10 I = 1,N
2406   10    X(I) = GN(0.,SIGMA(I))
2407         RETURN
2408         END


2409         SUBROUTINE NOISEV (T,CAPX,X,SIGMA,N,ND)
2410         DIMENSION CAPX(ND,ND),X(ND),SIGMA(ND)
2411         COMMON /IO/ NIN,NOUT,NTTY,NRUN,VER
2412         DATA NENTER /0/
2413 C       RETURNS A RANDOM VECTOR (X) WHOSE ELEMENTS X(I) HAVE VARIANCE
2414 C       CAPX(I,I), CAPX BEING THE COVARIANCE MATRIX FOR X, THAT IS,
2415 C       CAPX = E(X,XT).
2416 C       NOTE ... IT IS ASSUMED THAT CAPX IS A DIAGONAL MATRIX.
2417 C XXX   CAUTION XXX THIS ROUTINE HAS MEMORY..USE FOR ONLY ONE VARIABLE XX)
2418 C       THIS ROUTINE (NOISEV) USED FOR MEASUREMENT ERROR VECTOR (V).
2419 C       NOTE...BY REMOVING STMT 1 BELOW, THE ROUTINE WILL ACCOMODATE
2420 C       TIME-VARYING STATISTICS (IE, CAPX(T).NE.CONST, ETC.)
2421    1    IF (NENTER.EQ.NRUN) GO TO 5
2422         NENTER = NRUN
2423 C       THIS FORM FOR TIME INVARIANT STATISTICS SUCH THAT STANDARD
2424 C       DEVIATIONS ARE CALCULATED ONLY AT BEGINNING OF RUN.
2425 C       GENERAL CASE WOULD BE TO CALCULATE SIGMA(T) A FUNCTION OF TIME.
2426 C       DETERMINE STANDARD DEVIATIONS FIRST TIME THROUGH
2427         DO 2 I=1,N
2428    2    SIGMA(I) = SQRT(CAPX(I,I))
2429    5    DO 10 I = 1,N
2430   10    X(I) = GN(0.,SIGMA(I))
2431         RETURN
2432         END


2433         FUNCTION GN (MU,SIGMA)
2434 C       SUBROUTINE RETURNS A NORMALLY DISTRIBUTED (PSEUDO-) RANDOM NUMBER
2435 C       WITH MEAN (MU) AND STANDARD DEVIATION (SIGMA).
2436 C       THE ROUTINE USES (RAND(.)) WHICH IS TO RETURN A (PSEUDO-) RANDOM
2437 C       NUMBER WITH UNIFORM DISTRIBUTION ON THE OPEN INTERVAL (0,1).
2438 C
2439 C       REF..D. E. KNUTH, THE ART OF COMPUTER PROGRAMMING,
2440 C       VOL. 2, ADDISON-WESLEY(1969), PP. 103-104.
2441 C
2442         DATA NENTER /0/, KERNEL /0/
2443         REAL MU,SIGMA
2444         NENTER = NENTER + 1
```

```
      IF (NENTER.EQ.2) GO TO 2
    1 V1 = 2. * RANDOM(KERNEL) - 1.
      V2 = 2. * RANDOM(KERNEL) - 1.
      S = V1 * V1  +  V2 * V2
      IF (S.GE.1.) GO TO 1
          RAD = SQRT ((-2. * ALOG(S)) / S)
          GN = SIGMA * V1 * RAD  +  MU
          RETURN
    2     GN = SIGMA * V2 * RAD  +  MU
          NENTER = 0
          RETURN
      END


      FUNCTION RAND (IY)
C     ROUTINE RETURNS A (PSEUDO-) RANDOM NUMBER
C     UNIFORMLY DISTRIBUTED ON THE OPEN INTERVAL (0.,1.).
C     ROUTINE IS PORTABLE.  IE, IT SHOULD WORK ON ANY MACHINE.
C     (SEE REF FOR DETAILS.)
C
C     REF...FRITSCH, F. N., UNIVERSITY OF CALIFORNIA,
C     LAWRENCE LIVERMORE LABORATORY (PRIVATE COMMUNICATION), AND
C     INTERNAL DOCUMENT ... NUMERICAL MATHEMATICS SECTION NOTE NO. 66,
C     FEB. 7, 1973, UCLLL.
C
      DATA M2 /0/, ITWO /2/
      IF (M2 .NE. 0) GO TO 20
C     COMPUTE WORD SIZE OF MACHINE...
      M = 1
   10 M2 = M
      M = ITWO*M2
      IF (M .GT. M2) GO TO 10
      HALFM = M2
C     COMPUTE MULTIPLIER, INCREMENT, AND SCALE FACTOR...
      IA = 8*IFIX(HALFM*ATAN(1.)/8.) + 5
      IC = 2*IFIX(HALFM*(0.5-SQRT(3.)/6.)) + 1
      S = 0.5/HALFM
C     COMPUTE THE NEXT RANDOM NUMBER...
   20 IY = IY*IA + IC
      IF (IY/2 .GT. M2)  IY = (IY-M2)-M2
      IF (IY .LT. 0)     IY = (IY+M2)+M2
      RAND = FLOAT(IY)*S
      RETURN
      END


      SUBROUTINE UBAR (L,T,U,IU,UK,ND)
      DIMENSION UK(ND,3),IU(ND),U(ND)
C     SUBROUTINE RETURNS THE INPUT VECTOR (U(I,T),I=1,L)
C     IT USES EXTERNAL FUNCTION UI(,,,,,,) WHICH SETS EACH ELEMENT.
C     SEE (FUNCTION UI) LISTING FOR MEANING OF SWITCH (IU).  AND ARRAY
C     OF FUNCTION PARAMETERS (UK).
      EXTERNAL UI
      DO 1 I=1,L
    1 U(I) = UI(IU(I),I,UK,ND)
      RETURN
      END


      FUNCTION UI (IU,I,UK,ND)
C     SUBROUTINE RETURNS (UI) AN ELEMENT OF AN INPUT VECTOR WHICH IS
C     A FUNCTION OF TIME AS SELECTED BY (IU).  INCLUDED TIME FUNCTIONS
C     ARE LISTED BELOW.  PARAMETERS FOR THOSE FUNCTIONS ARE PASSED
C     THROUGH (UK(I,J)).  (I) IS THE VECTOR ELEMENT INDEX.
C     NOTE...FOLLOWING DIMENSION IS FOR MAX OF 3 PARAMETERS PER INPUT.
      DIMENSION UK(ND,3)
C     IU IS A SWITCH TO SELECT TYPE OF FORCING FUNCTION...SEE BELOW.
      IUP1 = IU + 1
      GO TO (1,2,3,4,5,6,7,8,9),IUP1
C     ZERO ELEMENT
    1 UI = 0.0
      RETURN
C     STEP INPUT OF MAGNITUDE UK(I,1)
    2 UI = UK(I,1)
      RETURN
C     RAMP INPUT OF GAIN UK(I,1) WITH INITIAL VALUE UK(I,2)
    3 UI = UK(I,1)* T  +  UK(I,2)
      RETURN
C     PARABOLIC INPUT
    4 UI = UK(I,1)*T*T  +  UK(I,2)*T  +  UK(I,3)
      RETURN
C     A*SIN(OMEGA*T + PHI) INPUT
    5 UI = UK(I,1)*SIN(UK(I,2)*T + UK(I,3))
      RETURN
C     GAUSSIAN NOISE INPUT WITH MEAN UK(I,1) AND STD DEV UK(I,2)
    6 UI = GN (UK(I,1),UK(I,2))
      RETURN
    7 CONTINUE
      RETURN
    8 CONTINUE
```

```
2529          RETURN
2530    9     CONTINUE
2531          RETURN
2532          END


2533          SUBROUTINE MATINPT (A,N,M,NAME,ND)
2534          DIMENSION A(ND,ND)
2535          COMMON /IO/ NIN,NOUT,NTTY,NRUN
2536          DO 1 I=1,N
2537    1     READ (NIN,101) (A(I,J),J=1,M)
2538  101     FORMAT (8E10.3)
2539          WRITE (NOUT,102)NAME
2540  102     FORMAT (/,1X,A7,13H MATRIX IS...,/)
2541          DO 2 I=1,N
2542    2     WRITE(NOUT,103) (A(I,J),J=1,M)
2543  103     FORMAT (10(1X,E10.3))
2544          RETURN
2545          END


2546          SUBROUTINE VECINPT (X,N,NAME,ND)
2547          DIMENSION X(ND)
2548          COMMON /IO/ NIN,NOUT,NTTY,NRUN
2549          READ (NIN,10 ) (X(I),I=1,N)
2550  101     FORMAT (8E10.3)
2551          WRITE (NOUT,102)NAME
2552  102     FORMAT (/,1X,A7,13H VECTOR IS...,/)
2553          WRITE(NOUT,103) (X(I),I=1,N)
2554  103     FORMAT (10(1X,E10.3))
2555          RETURN
2556          END


2557          SUBROUTINE MATOUTP (A,N,M,NAME,ND)
2558          DIMENSION A(ND,ND)
2559          COMMON /IO/ NIN,NOUT,NTTY,NRUN
2560          WRITE(NOUT,101)NAME
2561  101     FORMAT (/,1X,A7,13H MATRIX IS...,/)
2562          DO 1 I=1,N
2563    1     WRITE(NOUT,102)(A(I,J),J=1,M)
2564  102     FORMAT(10(1X,E10.3))
2565          RETURN
2566          END


2567          SUBROUTINE VECOUTP (X,N,NAME,ND)
2568          DIMENSION X(ND)
2569          COMMON /IO/ NIN,NOUT,NTTY,NRUN
2570          WRITE(NOUT,101)NAME
2571  101     FORMAT (/,1X,A7,13H VECTOR IS...,/)
2572          WRITE(NOUT,102)(X(I),I=1,N)
2573  102     FORMAT(10(1X,E10.3))
2574          RETURN
2575          END


2576          SUBROUTINE DEBUG (N,L,M,LL,T,TO,X,XH,G,Y,YH,E,W,V,P,PP,IOUT,ND)
2577 C        THIS ROUTINE USED TO GENERATE STRUNG-OUT LIST OF (ALMOST) ANY OF
2578 C        THE PROBLEM VARIABLES AS TIME PROCEEDS.  IT IS MAINLY MEANT FOR
2579 C        DEBUGGING PURPOSES SINCE THE FORM OF THE OUTPUT IS DIFFICULT TO
2580 C        INTERPRET.
2581          DIMENSION X(ND),XH(ND),G(ND,ND),Y(ND),YH(ND),E(ND),W(ND),V(ND),
2582         2          P(ND,ND),PP(ND,ND),IOUT(10)
2583          DIMENSION EQUALS(10)
2584          DATA EQUALS /10*1CH=/
2585          COMMON /IO/ NIN,NOUT,NTTY,NRUN
2586          IF(T.EQ.TO)WRITE(NOUT,101)NRUN
2587  101     FORMAT(30H1DEBUGGING OUTPUT IS AS FOLLOWS...RUN ,I2)
2588          WRITE(NOUT,103)(EQUALS(I),I=1,N)
2589  103     FORMAT(/,1X,10A10)
2590          WRITE(NOUT,102)T
2591  102     FORMAT(/,'T = ',E10.3,/)
2592 C        THE CODE FOR (IOUT(I),I=1,10) CAN BE DEDUCED FROM THE FOLLOWING
2593 C        TEN STATEMENTS.  IF A GIVEN (IOUT(I)) SS 1, ITS CORRESPONDING
2594 C        VECTOR OR MATRIX IS PRINTED AT EACH TIME STEP.
2595          IF(IOUT( 1).EQ.1)CALL VECOUTP (X,N,1HX,ND)
2596          IF(IOUT( 2).EQ.1)CALL VECOUTP (XH,N,2HXH,ND)
2597          IF(IOUT( 3).EQ.1)CALL MATOUTP (G,N,M,1HG,ND)
2598          IF(IOUT( 4).EQ.1)CALL VECOUTP (Y,M,1HY,ND)
2599          IF(IOUT( 5).EQ.1)CALL VECOUTP (YH,M,2HYH,ND)
2600          IF(IOUT( 6).EQ.1)CALL VECOUTP (E,N,6H(X-XH),ND)
2601          IF(IOUT( 7).EQ.1)CALL VECOUTP (W,LL,1HW,ND)
2602          IF(IOUT( 8).EQ.1)CALL VECOUTP (V,M,1HV,ND)
2603          IF(IOUT( 9).EQ.1)CALL MATOUTP (P,N,N,1HP,ND)
2604          IF(IOUT(10).EQ.1)CALL MATOUTP (PP,N,N,2HPP,ND)
2605          RETURN
2606          END
```

```
      SUBROUTINE OUTPUT3 (X,NAME,NCOL,N,TIME,TO,T1,T,ST
     2 XYPW1,XYPW2,TITLES,NTL,NAMEST,NCOLST,IMAX,JMAX,NI,NJ,NK)
C
C     ROUTINE VARIABLES ARE AS FOLLOWS...
C     X(J)              THE VECTOR OF LENGTH N...
C     N                 TO BE STORED FOR PLOTTING AT TIME...
C     TIME              WHERE TIME RUNS FROM INITIAL VALUE OF...
C     TO                TO FINAL VALUE OF...
C     T1                THE VARIOUS TIMES ARE STORED IN...
C     T(I)              THE PLOTTING VECTORS ARE STORED IN...
C     ST(I,J,K)         WHERE I = THE LAYER OF STORED VALUES OF THE VECTORS
C                       AT TIME T(I), J = THE ELEMENT INDEX ON X(J) AND
C                       K = THE NUMBER OF THE VECTOR STORED.  THUS...
C     IMAX              IS THE MAXIMUM NUMBER OF POINTS (IN TIME) PER PLOT,
C     JMAX(K)           IS A STORAGE ARRAY OF THE LENGTHS OF THE K VECTORS
C     NI,NJ,NK          ARE THE PHYSICAL DIMENSIONS OF THE APPROPRIATE ARRAYS
C                       IN THE CALLING PROGRAM.
C     NCOL              IS A SWITCH.  IT IS TO BE ZERO IF X IS A VECTOR,
C                       IT IS TO BE SET TO THE COLUMN NUMBER IF X IS
C                       A COLUMN OF A MATRIX (USED ONLY IN LABELLING)
C     NAME              IS A 9-CHARACTER HOLLERITH NAME FOR X USED FOR
C                       LABELLING (EG, NAME = 3H XK)...
C     NOTE   ...        IMAX.LE.NI, JMAX(K).LE.NJ, KMAX.LE.NK.
C
      DIMENSION X(NJ),T(NI),ST(NI,NJ,NK),JMAX(NK),NAMEST(NK),TITLES(4,8)
      DIMENSION XYPW1(NI),XYPW2(NI),NCOLST(NK)
      DATA K/1/
      DATA I/0/
      COMMON /IO/ NIN,NOUT,NTTY,NRUN
C     IF A PROBLEM MATRIX HAS BECOME SINGULAR SO THAT THE PRESENT RUN
C     IS TO BE ABORTED, GO TO DUMP OUTPUT UP TO PRESENT TIME AND
C     REINITIALIZE POINTERS FOR NEXT PROBLEM.
      IF(NAME.EQ.10H  SINGULAR)GO TO 11
      IF(TIME.NE.TO)                GO TO 1
C     INITIALIZE ROW LENGTHS FOR VARIOUS VECTORS TO BE PLOTTED(JMAX(K)).
C     ALSO, DETERMINE MAXIMUM NUMBER OF VECTORS TO BE PLOTTED (KMAX).
C     STORE VECTOR NAMES AS THEY COME DOWN.  STORE (NAME) IN (NAMEST).
C     STORE (NCOL) IN (NCOLST) TO SIGNIFY WHETHER (X) IS A COLUMN OF A
C     MATRIX OR JUST A SIMPLE VECTOR.
      KMAX = K
      JMAX(K) = N
      NAMEST(K) = NAME
      NCOLST(K) = NCOL
      TM1 = TIME
      IF(K.NE.1)                    GO TO 8
      GO TO 2
    1 IF(TIME.EQ.TM1)               GO TO 8
C     START A NEW LAYER AT NEXT TIME.
C     TM1 IS USED AS A MEMORY ELEMENT FOR SWITCHING.
C     IF TM1.EQ.TIME, THEN IT MEANS THAT THIS IS NOT THE FIRST VECTOR TO
C     BE STORED IN THE SEQUENCE OF CALLS TO (OUTPUT3).  IF TM1.NE.TIME,
C     (BUT ACTUALLY IT EQUALS THE PREVIOUS TIME), IT MEANS (TIME) WAS
C     JUST INCREMENTED IN THE CALLING PROGRAM SUCH THAT A NEW LAYER
C     SHOULD BE STARTED IN STORING THE VECTORS (THUS, SET K=1, I=I+1
C     AND T(I)=TIME).
      K = 1
      TM1 = TIME
    2 IF(I.NE.IMAX)                 GO TO 7
C     I IS AT THE ALLOWABLE MAXIMUM OF TIME POINTS PER PLOT (IMAX).
C     DO THE PLOTTING...
      DO 4 K = 1,KMAX
      JMAXK = JMAX(K)
      DO  3 J = 1,JMAXK
      CALL XYPLOT (T,ST(1,J,K),I,J,XYPW1,XYPW2,
     2 NAMEST(K),NCOLST(K),TITLES,NTL,NRUN,NOUT,NI)
    3 CONTINUE
      CALL TABULAR(T,ST(1,1,K),I,JMAX(K),NJ,
     2 NAMEST(K),NCOLST(K),TITLES,NTL,NRUN,NOUT,NI)
    4 CONTINUE
C     COPY PRESENT LAYER INTO FIRST LAYER FOR CONTINUATION PLOT...
      DO 6 K = 1,KMAX
      JMAXK = JMAX(K)
      DO  5 J = 1,JMAXK
    5 ST(1,J,K) = ST(IMAX,J,K)
    6 CONTINUE
C     RESET  INDICES TO POINT TO FIRST PLOTTED VECTOR OF FIRST LAYER
      K = 1
      I = 1
      T(I) = T(IMAX)
    7 CONTINUE
C     AT START OF NEW LAYER (NEW TIME).  INCREMENT I AND STORE T(I)...
      I = I + 1
      T(I) = TIME
    8 CONTINUE
C     STORE PRESENT VECTOR X(J) INTO KTH VECTOR POSITION IN ITH LAYER
C     OF (ST)...
      JMAXK = JMAX(K)
      DO 10 J = 1,JMAXK
   10 ST(I,J,K) = X(J)
      IF(TIME.LT.T1)                GO TO 20
```

```
      IF(K.LT.KMAX)                GO TO 20
C     AT THE END OF TIME INTERVAL (TO,TI) FOR THE FINAL VECTOR.
C     DO THE PLOTTING...
 11   CONTINUE
      DO 16 K = 1,KMAX
      JMAXK = JMAX(K)
      DO 15 J = 1,JMAXK
      CALL XYPLOT (T,ST(1,J,K),1,J,XYPW1,XYPW2,
     2 NAMEST(K),NCOLST(K),TITLES,NTL,NRUN,NOUT,NI)
 15   CONTINUE
      CALL TABULAR(T,ST(1,1,K),1,JMAX(K),NJ,
     2 NAMEST(K),NCOLST(K),TITLES,NTL,NRUN,NOUT,NI)
 16   CONTINUE
      WRITE(5)1
      WRITE(5)(T(II),II=1,I)
      WRITE(5)((ST(II,J,K),II=1,I)
C     RESET INDICES FOR NEW PROBLEM AS IN DATA STATEMENTS...
      K = 1
      I = 0
      GO TO 99
 20   CONTINUE
C     ADVANCE PLOT VECTOR INDEX FOR NEXT CALL...
      K = K + 1
 99   RETURN
      END


      SUBROUTINE TABULAR (T,X,NT,N,NJ,
     2 NAME,NCOL,TITLES,NTL,NRUN,NOUT,NI)
C     ROUTINE GENERATES A TABULAR LISTING OF X(T), X AN N-VECTOR.
C     ROUTINE VARIABLES ARE AS FOLLOWS...
C     X(I,J)           THE ARRAY OF N-VECTORS AS A FUNCTION OF TIME
C                      STORED ROW-WISE.
C     T(I)             THE CORRESPONDING TIMES FOR WHICH ELEMENTS OF X
C                      WERE STORED.
C     NT               NUMBER OF POINTS IN TIME FOR VECTORS STORED.
C     NAME             A 3-CHARACTER HOLLERITH NAME FOR LABELLING.
C     TITLES(4,8)      DESCRIPTIVE INFORMATION.
C     NOUT             LOGICAL UNIT NUMBER FOR OUTPUT.
C     NRUN             RUN NUMBER.
C     NTL              NUMBER OF TITLE CARDS.
C     NI,NJ            DIMENSIONS OF X(NI,NJ) AND T(NI) IN CALLING PROGRAM.
      DIMENSION X(NI,NJ),T(NI),TITLES(4,8),LABEL(10)
      DO 1 I = 1,N
 1    LABEL(I) = NAME
      WRITE(NOUT,101)NRUN
 101  FORMAT(9H1RUN NO. ,I2,/)
      IF(NTL.EQ.0) GO TO 6
      DO 5 I = 1,NTL
 5    WRITE(NOUT,105)(TITLES(I,J),J=1,8)
 105  FORMAT(1X,8A10)
 6    CONTINUE
      IF(NCOL.NE.0) GO TO 10
      WRITE(NOUT,102)((LABEL(I),I),I=1,N)
 102  FORMAT(/,11H        TIME,10(4X,A3,1H(,I2,1H)))
      GO TO 20
 10   WRITE(NOUT,120)((LABEL(I),I,NCOL),I=1,N)
 120  FORMAT(/,11H        TIME,10(1X,A3,1H(,I2,1H,,I2,1H)))
 20   CONTINUE
      DO 2 I = 1,NT
 2    WRITE(NOUT,104)T(I),(X(I,J),J=1,N)
 104  FORMAT(11(1X,E10.3))
      RETURN
      END


      SUBROUTINE XYPLOT (XIN,YIN,NUMPTS,NROW,X,Y,
     2 NAME,NCOL,TITLES,NTL,NRUN,NOUT,ND)
C
C     REF.. MCCUE, H. K., UNIVERSITY OF CALIFORNIA,
C     LAWRENCE LIVERMORE LABORATORY (PRIVATE COMMUNICATION), AND
C     PHD. DISSERTATION, UNIVERSITY OF CALIFORNIA, BERKELEY, 1975.
C
      DIMENSION XIN(ND),YIN(ND),X(ND),Y(ND)
      DIMENSION POINTS(101),BUT(6),TITLES(4,8)
      IF(NUMPTS.LT.2)GO TO 999
C COPY INPUT VECTORS (XIN,YIN) INTO WORKING STORAGE (X,Y)
      DO 1 I=1,NUMPTS
      X(I) = XIN(I)
      Y(I) = YIN(I)
 1    CONTINUE
C WRITE OUT TITLE CARDS
      WRITE(NOUT,6)
 6    FORMAT(1H1)
      DO 3 I=1,4
      GO TO (301,302,303,303),I
 301  IF(I.LE.NTL)WRITE(NOUT,3001)NRUN,(TITLES(I,J),J=1,8)
 3001 FORMAT(9X,8HRUN NO. ,I2,2X,8A10)
      IF(I.GT.NTL)WRITE(NOUT,3011)NRUN
 3011 FORMAT(9X,8HRUN NO. ,I2)
```

```
      GO TO 3
C     (NROW) IS ROW ELEMENT NUMBER
C     (NCOL) IS COLUMN ELEMENT NUMBER IF (YIN) IS A COLUMN OF A MATRIX,
C            IT IS ZERO IF (YIN) IS A SIMPLE VECTOR.
302   IF((I.LE.NTL).AND.(NCOL.NE.0))
     2     WRITE(NOUT,3021)NAME,NROW,NCOL,(TITLES(I,J),J=1,8)
3021  FORMAT(2X,A3,1HI,I2,1H,,I2,1H),2X,8A10)
      IF((I.LE.NTL).AND.(NCOL.EQ.0))
     2     WRITE(NOUT,3022)NAME,NROW,(TITLES(I,J),J=1,8)
3022  FORMAT(2X,A3,1HI,I2,1H),2X,8A10)
      IF((I.GT.NTL).AND.(NCOL.NE.0))
     2     WRITE(NOUT,3023)NAME,NROW,NCOL
3023  FORMAT(3X,A3,1HI,I2,1H,,I2,1H))
      IF((I.GT.NTL).AND.(NCOL.EQ.0))
     2     WRITE(NOUT,3024)NAME,NROW
3024  FORMAT(3X,A3,1HI,I2,1H))
      GO TO 3
303   IF((I.LE.NTL).WRITE(NOUT,3031)(TITLES(I,J),J=1,8)
3031  FORMAT(13X,8A10)
      IF((I.GE.NTL)WRITE(NOUT,5)
3     CONTINUE
      WRITE(NOUT,5)
5     FORMAT(1H )
C
C  REORDER BY THE Y AXIS.
C
C  SAVE FOR MAX
      I=1
20    CONTINUE
      JJ=1
      YMAX=Y(1)
      DO 10 J=1,NUMPTS
      IF(Y(J).LE.YMAX)GO TO 10
      YMAX=Y(J)
      JJ=J
10    CONTINUE
C  INTERCHANGE
      YY=Y(I)
      XX=X(I)
      Y(I)=Y(JJ)
      X(I)=X(JJ)
      Y(JJ)=YY
      X(JJ)=XX
      I=I+1
      IF(I.EQ.NUMPTS)GO TO 30
      GO TO 20
30    CONTINUE
C  SAVE FOR MIN/MAX OF X AND Y.
      XMIN=X(1)
      XMAX=X(1)
      YMIN=Y(1)
      YMAX=Y(1)
      DO 2 I=1,NUMPTS
      IF(X(I).LT.XMIN)XMIN=X(I)
      IF(X(I).GT.XMAX)XMAX=X(I)
      IF(Y(I).LT.YMIN)YMIN=Y(I)
      IF(Y(I).GT.YMAX)YMAX=Y(I)
2     CONTINUE
C  RESET THE ENV POINTS.
      CALL ENDPTS(XMIN,XMAX)
      CALL ENDPTS(YMIN,YMAX)
C  CALCULATE DELX AND DELY.
      DELX=(XMAX-XMIN)/100.0
      DELY=(YMAX-YMIN)/50.0
C  CALCULATE THE PLOT
      KK=ABS(XMIN)/DELX+1.0
      IZERO=0
      IF((XMIN.LE.0.0).AND.(XMAX.GE.0.0))IZERO=1
      ICOUNT=10
      LIST=1
      DO 104 I=1,51
      XI=I
      YZ2=YMAX-XI*DELY
      YZ1=YZ2+DELY
      IAA=0
      IF((YZ1.GE.0.0).AND.(YZ2.LE.0.0))IAA=1
      DO 10; J=1,101
      POINTS(J)=1H
101   IF(ICOUNT.NE.10)GO TO 105
      DO 106 J=1,101,2
      POINTS(J)=1H.
106   CONTINUE
105   POINTS(  1)=1H.
      POINTS( 21)=1H.
      POINTS( 41)=1H.
      POINTS( 61)=1H.
      POINTS( 81)=1H.
      POINTS(101)=1H.
      IF(IZERO.EQ.1)POINTS(KK)=1HI
      IF(IAA.NE.1)GO TO 107
```

```
      DO 136 J=1,101
      POINTS(J)=1H
  136 CONTINUE
  137 YLOW=YMAX-XI*DELY
      CONTINUE
  102 IF(LIST.GT.NUMPTS)GO TO 110
      IF(Y(LIST).LT.YLOW)GO TO 110
      K=(X(LIST)-XMIN)/DELX+1.0
      POINTS(K)=1HX
      LIST=LIST+1
      GO TO 102
  110 CONTINUE
      IF(ICOUNT.EQ.10)GO TO 112
      ICOUNT=ICOUNT+1
      WRITE(NOUT,111)(POINTS(J),J=1,101)
  111 FORMAT(15X,101A1)
      GO TO 100
  112 CONTINUE
      YY=YLOW-DELY
      ICOUNT=1
      IF((YY.GT.-1.0E-9).AND.(YY.LT.1.0E-9))YY=0.0
      WRITE(NOUT,113)YY,(POINTS(J),J=1,101)
  113 FORMAT(2X,E11.4,2X,101A1)
  100 CONTINUE
      DO 121 I=1,6
      XI=I-1
      BUT(I)=XMIN+20.0*DELX*XI
      IF((BUT(I).LT.1.0E-9).AND.(BUT(I).GT.-1.0E-9))BUT(I)=0.0
  121 CONTINUE
      WRITE(NOUT,122)(BUT(J),J=1,6)
  122 FORMAT(/,10X,6(E10.3,10X))
      WRITE(NOUT,202)
  202 FORMAT(56X,20HTIME (DIMENSIONLESS))
  999 CONTINUE
      RETURN
      END


      SUBROUTINE ENDPTS(XMIN,XMAX)
C THIS SUBROUTINE RESETS THE END POINTS OF PLOT.
C
C     REF...MCCUE, H. K., UNIVERSITY OF CALIFORNIA,
C     LAWRENCE LIVERMORE LABORATORY (PRIVATE COMMUNICATION), AND
C     PHD. DISSERTATION, UNIVERSITY OF CALIFORNIA, BERKELEY, 1975.
C
      DIMENSION A(38)
      DATA (A(I),I=1,38)/0.0,0.1,0.25,0.50,0.75,1.0,1.1,1.25,1.50,1.75,
     2.00,2.50,3.00,3.50,4.00,4.50,5.0,6.0,7.0,8.0,9.0,10.0,11.,12.5,
     15.,17.5,20.,25.,30.,35.,40.,45.,50.,60.,70.,80.,90.,100./
C CHECK XMIN/XMAX TERMS.
      IF(XMIN.NE.XMAX)GO TO 1
      XMIN=XMIN-1.0
      XMAX=XMAX+1.0
      GO TO 999
    1 CONTINUE
      DEL=XMAX-XMIN
      IF(DEL.GT.0.0)GO TO 2
      XX=XMAX
      XMAX=XMIN
      XMIN=XX
      DEL=-DEL
    2 CONTINUE
C DEL IS POSITIVE AT THIS POINT.
      VALUE=1.0
      IF(DEL.LE.1.0)GO TO 10
    5 CONTINUE
      IF(DEL.LT.VALUE)GO TO 20
      VALUE=VALUE*10.0
      GO TO 5
   10 CONTINUE
      IF(DEL.GE.VALUE)GO TO 11
      VALUE=VALUE*0.1
      GO TO 10
   11 VALUE=VALUE*10.0
   20 CONTINUE
      XX=XMIN/VALUE
      IXX=XX
      XX=IXX
      XX=XX*10.0
      XXMIN=XMIN*10.0/VALUE-XX
      XXMAX=XMAX*10.0/VALUE-XX
      IF(XXMIN.EQ.0.0)GO TO 30
      IF(XXMIN.LT.0.0)GO TO 35
C XXMIN IS POSITIVE.
      DO 32 I=2,38
      AAA=A(I)
      IF(XXMIN.LT.AAA)GO TO 33
   32 CONTINUE
   33 I=I-1
      XXMIN=A(I)
```

```
2961          GO TO 30
2962    35    CONTINUE
2963    C XXMIN IS NEGATIVE.
2964          XXMIN=-XXMIN
2965          DO 36 I=2,38
2966          AAA=A(I)
2967          IF(XXMIN.LT.AAA)GO TO 37
2968    36    CONTINUE
2969    37    XXMIN=-A(I)
2970    30    CONTINUE
2971          IF(XXMAX.EQ.0.0)GO TO 40
2972          IF(XXMAX.LT.0.0)GO TO 45
2973    C XXMAX IS POSITIVE
2974          DO 42 I=2,38
2975          AAA=A(I)
2976          IF(XXMAX.LE.AAA)GO TO 43
2977    42    CONTINUE
2978    43    XXMAX=A(I)
2979          GO TO 40
2980    45    CONTINUE
2981    C XXMAX IS NEGATIVE.
2982          XXMAX=-XXMAX
2983          DO 46 I=2,38
2984          AAA=A(I)
2985          IF(XXMAX.LE.AAA)GO TO 47
2986    46    CONTINUE
2987    47    I=I-1
2988          XXMAX=-A(I)
2989    40    CONTINUE
2990    C SOLVE FOR NEW END POINTS.
2991          XMIN=(XX+XXMIN)*VALUE/10.0
2992          XMAX=(XX+XXMAX)*VALUE/10.0
2993    999   CONTINUE
2994          RETURN
2995          END
```

APPENDIX G. DESCRIPTIONS AND LISTINGS OF POSTPROCESSOR PROGRAMS

All of the postprocessor programs listed in this Appendix have as their sole inputs the binary (unformatted) intermediate disc files, PFILE or TFILE, generated by PROGRAM KALMAN; see Figures F.1 and F.2 for their relationships to KALMAN and their own output files.

CONTOUR generates contour plots of the surfaces $[P_K^K(z_K)]_{11}$ at all measurement times t_K. The idea for the format of the plots was taken from Case Study 26 in McCracken [83]; the coding was this author's own.

POFT computes and plots surfaces for $\mathrm{Tr}[P_{K+N}^K(z_K)]$ for increasing values of time t_{K+N}. The particularly efficient algorithms for the evaluation of the trace function, as in subroutines FVAL and PVAL, are called to the readers attention; the amount of computation involved in generating the (51 x 81) point grids in these contour plots grows enormously with the size of the problem such that computational efficiency is of prime importance in their generation.

PELEM plots the contour surfaces of the diagonal elements of the covariance matrices, $[P_K^K(z_K)]_{ii}$, $i = 1,2,\ldots,n$. They show the decomposition of the trace of that matrix which led to the fundamental result for the infrequent sampling problem of Conclusion II.

SIGMAT plots the family of curves for $\sigma^2_{K+N}(z_K^*,z)$ as functions of the position z in the one-dimensional medium for a set of consecutive times $t_{K+N} = (t_K, t_K + \gamma, t_K + 2\gamma, \ldots)$, where γ is selected at the teletype. This routine was instrumental in showing the asymptotic movement of the position of maximum variance in the output estimate with time; see (6.54).

MAXTIME was used to compare the two performance criteria $\mathrm{Tr}[P_K^K(z_K)]$ and $[P_K^K(z_K)]_{11}$. It showed that minimizing the trace at the time of the

measurement is not optimal, whereas minimizin its first element is optimal for large time.

POSTPLT is used in various places to plot families of curves as functions of time resulting from multiple runs in KALMAN. Doing graphical displays with such a "postprocessor", that is, a program which operates on data generated by another (usually larger) program, was found to have a number of programming and computational advantages. Among them were small program size, ease of execution and versatility.

POSTFP was used to plot sections through the $[\underset{\sim}{P}^K_K(\underset{\sim}{z}_K)]_{11}$ surfaces in the study of the sensitivity of the optimal monitoring problem results to dimensionality of the model used in the monitor.

POSTSP plots $\sigma^2_K(\underset{\sim}{z}^*_K, z)$ as functions of z for monitor models of various dimensions.

Numerous extensions of the programs listed here can be conceived. Among them is the use of the various plotters in conjunction with other programs; the basic plotting routines are quite versatile in that sense. In the case of the contour plots, where the dimension of the measurement vector $\underset{\sim}{y}$ must be $m \equiv 2$, an obvious refinement is to replace the general purpose matrix inversion package with a simplified algorithm for inversion of the statistics matrix

$$\left[\underset{\sim}{T}^K_{K+N}\right]^{-1} \equiv \left[\underset{\sim}{C}(\underset{\sim}{z}_{K+N})\underset{\sim}{P}^K_{K+N}(\underset{\sim}{z}_K)\underset{\sim}{C}(\underset{\sim}{z}_{K+N})^T + \underset{\sim}{V}\right]^{-1}$$

in the covariance matrix correction algorithms; for these cases, $\underset{\sim}{T}^K_{K+N}$ is a (2×2) matrix.

```
      PROGRAM CONTOUR (PFILE,TAPE2=PFILE,COUT,TAPE3=COUT)
      CALL CHANGE(2H*C)
      CALL CREATE(4HCOUT,4000B,SWT)
      NIN = 2
      NOUT = 3
C
      DIMENSION A(10,10),P(10,10),CAPV(10,10),WKP1(10,10),WSS(10,10)
      DIMENSION CAPW(10,10)
      DIMENSION ZDUM(10)
      ZMAX = 1.0
      COMMON /ERROR/ N,M,ZMAX,A,P,CAPV,WKP1,WSS,ISING
C
      DIMENSION F(51,81),X(2),S(19),SLINE(81),SYMB(9)
      DATA S/ 1H ,1H1,1H ,1H2,1H ,1H3,1H ,1H4,1H ,1H5,
     2        1H ,1H6,1H ,1H7,1H ,1H8,1H ,1H9,1H /
      DATA SYMB / 1H1,1H2,1H3,1H4,1H5,1H6,1H7,1H8,1H9 /
      DIMENSION TITLES(4,8),BORD(51),SCALEH(51),SCALEV(11),SAMPLE(10)
      DATA BORD / 1H+,1*1H-,1H+,4*1H-,1H+,4*1H-,1H+,4*1H-,1H+,4*1H-,
     2 1H+,4*1H-,1H+,4*1H-,1H+,4*1H-,1H+,4*1H-,1H+,4*1H-,1H+,4*1H-,
     3 1H+ /
      DATA SCALEV/10H          ,1C +,4*10H                ,10H      0.9 +,
     1 2*10H                  ,10H      0.8 +,4*10H                ,10H      0.7 +,
     2 4*10H                  ,10H      0.6 +,2*10H                ,10H (Z(K)12.5,
     3 4   10H                ,10H      0.5 +,
     4 4*10H                  ,10H      0.4 +,4*10H                ,10H      0.3 +,
     5 4*10H                  ,10H      0.2 +,4*10H                ,10H      0.1 +,
     6 7*10H                  ,10H      0.0 */
      DATA SCALEV /8H0.0      ,8H0.1     ,8H0.2     ,8H0.3     ,
     2 8H0.4     ,8H0.5     ,8H0.6     ,8H0.7     ,8H0.8     ,
     3 8H0.9     ,3H1.0/
      DATA SAMPLE / 8HZEROETH ,
     1              8HFIRST   ,8HSECOND  ,8HTHIRD   ,8HFOURTH  ,
     2              8HFIFTH   ,8HSIXTH   ,8HSEVENTH ,8HEIGHTH  ,
     3              8HNINTH   /
      DIMENSION BORH(81)
      DATA BORH/1H+,7*1H-,1H+,7*1H-,1H+,7*1H-,1H+,7*1H-,1H+,7*1H-,1H+,7*1H-,
     2 1H+,7*1H-,1H+,7*1H-,1H+,7*1H-,1H+,7*1H-,1H+,7*1H-,1H+,7*1H-,1H+/
      NL = 19
      NX = 80
      NY = 50
      NXP1 = NX + 1
      NYP1 = NY + 1
C     SET CONTOUR PLOT LIMITS
      XMIN = 0.
      XMAX = ZMAX
      YMIN = 0.
      YMAX = ZMAX
      DX = (XMAX - XMIN)/NX
      DY = (YMAX - YMIN)/NY
 3 00 CONTINUE
      READ(NIN,1,END=99)N,M,LL,NTL,ID,T1,LIMIT
      IF(N.LT.0) GO TO 99
      READ(NIN,1)((A(I,J),J=1,N),I=1,N)
      IF(ID.NE.0)READ(NIN,1)((P(I,J),I=1,N),I=1,N)
      IF(ID.EQ.0)READ(NIN,1)((P(I,J),J=1,N),I=1,N)
      READ(NIN,1)((CAPV(I,J),J=1,LL),I=1,LL)
      READ(NIN,1)((CAPW(I,J),J=1,M),I=1,M)
      IF(NTL.EQ.0)READ(NIN,2)((TITLES(I,J),J=1,8),I=1,NTL)
 3    CONTINUE
      READ(NIN,1)IORD,T,ERRLIM,DT
      IF(IORD.LT.0) GO TO 3000
      READ(NIN,1)((P(I,J),J=1,N),I=1,N)
      IF(NOT.GT.0)READ(NIN,1)(ZDUM(I),I=1,M)
      IF(NOP.GT.0)READ(NIN,1)(ZDUM(I),I=1,M)
      X(1) = XMIN
      X(2) = YMIN
      CALL EVAL (X,FMIN)
      FMAX = FMIN
      DO 2 I=1,NXP1
C     X(1) INCREMENTALLY, X(2) VERTICALLY...
      X(2) = YMIN + (I-1)*DY
      DO 2 J=1,NXP1
      X(1) = XMIN + (J-1)*DX
      CALL EVAL (X,F(I,J))
      IF(F(I,J).LT.FMIN)FMIN = F(I,J)
      IF(F(I,J).GT.FMAX)FMAX = F(I,J)
 1    CONTINUE
 2    CONTINUE
      DF = (FMAX - FMIN)/NL
      NOPP1 = NOP+1
      WRITE(NOUT,101)T,(TITLES(1,I),I=1,8),SAMPLE(NOPP1),
     2                 (TITLES(2,J),J=1,8)
101   FORMAT(*1*,10X,*CONTOUR PLOT OF (P(K,K)/Z(K))11 AS A FUNCTION OF*
     2,* Z(K)11 HORIZ AND Z(K)12 VERT*,9X,*TIME   *,E11.4,/,
     3 11X,8A10,9X,A8,*MEASUREMENT*,/
     4 11X,8A10,/)
      WRITE(NOUT,107)BORH
107   FORMAT(10X,81A1,9X,16(1H=))
      DO 1000 I=1,NYP1
      DO 9 J=1,NXP1
      DO 5 K=1,NL
```

```
      IF((FMIN+K*DF).GT.F(NYP1+1-I,J))GO TO 6
  5   CONTINUE
  6   SLINE(J) = S(K)
      IF((F(NYP1+1-I,J)).EQ.FMIN) SLINE(J) = 1H*
      IF((F(NYP1+1-I,J)).EQ.FMAX) SLINE(J) = 1HO
  9   CONTINUE
      IF(I.GT.7)GO TO 280
      GO TO(21,22,23,24,25,26,27),I
 21   WRITE(NOUT,201)SCALEH(I),SLINE,BDR(I)
201   FORMAT(A10,81A1,A1,8X,* CONTOUR LEVELS*)
      GO TO 1000
 22   WRITE(NOUT,202)SCALEH(I),SLINE,BDR(I)
202   FORMAT(A10,81A1,A1,8X,*  AND SYMBOLS*)
      GO TO 1000
 23   WRITE(NOUT,203)SCALEH(I),SLINE,BDR(I)
203   FORMAT(A10,81A1,A1,8X,16(1H=))
      GO TO 1000
 24   WRITE(NOUT,204)SCALEH(I),SLINE,BDR(I)
204   FORMAT(A10,81A1,A1,8X,*SYMB LEVEL RANGE*)
      GO TO 1000
 25   WRITE(NOUT,203)SCALEH(I),SLINE,BDR(I)
      GO TO 1000
 26   WRITE(NOUT,206)SCALEH(I),SLINE,BDR(I),FMAX
206   FORMAT(A10,81A1,A1,8X,4H (O),E11.4)
      GO TO 1000
 27   WRITE(NOUT,207)SCALEH(I),SLINE,BDR(I)
207   FORMAT(A10,81A1,A1,8X,16(1H-))
      NSKIP = 1
      NLEVEL = 9
      GO TO 1000
280   IF(I.GT.34)GO TO 350
      GO TO(28,28,29),NSKIP
 28   FLEVEL = FMIN + (2*NLEVEL+1-NSKIP)*DF
      WRITE(NOUT,208)SCALEH(I),SLINE,BDR(I),SYMB(NLEVEL),FLEVEL
208   FORMAT(A10,81A1,A1,8X,* (*,A1,*)*,E11.4)
      NSKIP = NSKIP+1
      GO TO 1000
 29   NSKIP = 1
      NLEVEL = NLEVEL - 1
      WRITE(NOUT,207)SCALEH(I),SLINE,BDR(I)
      GO TO 1000
350   LINE = I - 34
      GO TO(35,36,37,38,39,40,36,42,43,44,45,36,47,48,44,50,51,52),LINE
 35   WRITE(NOUT,235)SCALEH(I),SLINE,BDR(I),FMIN
235   FORMAT(A10,81A1,A1,8X,4H (*),E11.4)
      GO TO 1000
 36   WRITE(NOUT,203)SCALEH(I),SLINE,BDR(I)
      GO TO 1000
 37   WRITE(NOUT,237)SCALEH(I),SLINE,BDR(I)
237   FORMAT(A10,81A1,A1,8X,*ESTIMATION=)
      GO TO 1000
 38   WRITE(NOUT,238)SCALEH(I),SLINE,BDR(I)
238   FORMAT(A10,81A1,A1,8X,*ERROR CRITERION=)
      GO TO 1000
 39   WRITE(NOUT,239)SCALEH(I),SLINE,BDR(I)
239   FORMAT(A10,81A1,A1,8X,*CONSTRAINT ==)
      GO TO 1000
 40   WRITE(NOUT,240)SCALEH(I),SLINE,BDR(I),ERRLIM
240   FORMAT(A10,81A1,A1,12X,E11.4)
      GO TO 1000
 42   WRITE(NOUT,242)SCALEH(I),SLINE,BDR(I)
242   FORMAT(A10,81A1,A1,8X,*SOURCE INPUT=)
      GO TO 1000
 43   WRITE(NOUT,243)SCALEH(I),SLINE,BDR(I)
243   FORMAT(A10,81A1,A1,8X,*COVARIANCE  (W)==)
      GO TO 1000
 44   WRITE(NOUT,244)SCALEH(I),SLINE,BDR(I)
244   FORMAT(A10,81A1,A1)
      GO TO 1000
 45   WRITE(NOUT,245)SCALEH(I),SLINE,BDR(I),CAPW(1,1)
245   FORMAT(A10,81A1,A1,8X,*(   *,E11.4,*)*)
      GO TO 1000
 47   WRITE(NOUT,247)SCALEH(I),SLINE,BDR(I)
247   FORMAT(A10,81A1,A1,8X,*MEASUREMENT=)
      GO TO 1000
 48   WRITE(NOUT,248)SCALEH(I),SLINE,BDR(I)
248   FORMAT(A10,81A1,A1,8X,*ERROR COVAR (V)==)
      GO TO 1000
 50   WRITE(NOUT,250)SCALEH(I),SLINE,BDR(I),CAPV(1,1),CAPV(1,2)
250   FORMAT(A10,81A1,A1,8X,*(*,F0.3,4X,F0.3,*)*)
      GO TO 1000
 51   WRITE(NOUT,250)SCALEH(I),SLINE,BDR(I),CAPV(2,1),CAPV(2,2)
      GO TO 1000
 52   WRITE(NOUT,203)SCALEH(I),SLINE,BDR(I)
1000  CONTINUE
      WRITE(NOUT,107)BDRH
      WRITE(NOUT,253)SCALEV
253   FORMAT(/,9X,11A8,/,51X,*(Z(K))*)
      CALL MATOUTP (P,N,N,1HP,NOUT,10)
      GO TO 3
```

```
      99    CALL EXIT(1)
            END

            SUBROUTINE FVAL (Z,P11)
      C     SEE PROGRAM KALMAN FOR THIS ROUTINE...
            END

            SUBROUTINE MATOUTP (A,N,M,NAME,NOUT,ND)
            DIMENSION A(ND,ND)
            WRITE(NOUT,101)NAME
      101   FORMAT(/,10X,A4,13H MATRIX IS.../)
            DO 1 I=1,N
      1     WRITE(NOUT,102)(A(I,J),J=1,M)
      102   FORMAT(10X,10(E10.3,1X))
            RETURN
            END

            SUBROUTINE INVERSE (NN,A,AINV,IERROR)
      C     SEE PROGRAM KALMAN FOR THIS ROUTINE...
            END

            SUBROUTINE DECOMP (NN,A,UL,SCALES,IPS,IERROR,ND)
      C     SEE PROGRAM KALMAN FOR THIS ROUTINE
            END

            SUBROUTINE SOLVE (NN,UL,B,X,IPS,ND)
      C     SEE PROGRAM KALMAN FOR THIS ROUTINE...
            END

            SUBROUTINE IMPRUV (NN,A,UL,B,X,R,DX,IPS,DIGITS,IERROR,ND)
      C     SEE PROGRAM KALMAN FOR THIS ROUTINE...
            END
```

```
      PROGRAM POFT (PFILE,TAPE2=PFILE,PTOUT,TAPE3=PTOUT)
C     SET (NPLOT) TO THE NUMBER OF THE MEASUREMENT FOR WHICH THE CONTOUR
C     PLOTS ARE DESIRED (1, 2,...).  SET IT TO ZERO (0) IF PLOTS
C     ARE DESIRED AFTER ALL MEASUREMENTS.  CAUTION, THERE ARE (IIMAX)
C     PLOTS ASSOCIATED WITH EACH MEASUREMENT.  EACH SPACED (KNS=DT)
C     UNITS OF TIME AFTER (T(K)) FOR EACH MEASUREMENT.  GETS COSTLY
      CALL CHANGE (2H+P)
      CALL CREATE (5HPTOUT,40000,SWT)
      NIN = 2
      NOUT = 3
      NTTY = 59
      DIMENSION A(10,10),WKP1(10,10),CAPV(10,10),P(10,10)
      DIMENSION CAPW(10,10)
      DIMENSION WSS(10,10)
      DIMENSION ZDUM(10)
      ZMAX = 1.0
      COMMON /PROB/ N,M,ZMAX,P,CAPV,ISING
      COMMON /PROB2/ A,WKP1,DT,T
C
      DIMENSION F(51,81),X(2),S(19),SLINE(81),SYMB(9)
      DATA S / 1H ,1H1,1H ,1H2,1H ,1H3,1H ,1H4,1H ,1H5,
     2         1H ,1H6,1H ,1H7,1H ,1H8,1H ,1H9,1H /
      DATA SYMB / 1H1,1H2,1H3,1H4,1H5,1H6,1H7,1H8,1H9 /
      DIMENSION TITLES(4,8),BDR(51),SCALEH(51),SCALEV(11),SAMPLE(10)
      DATA BDR / 1H+,4*1H-,1H+,4*1H-,1H+,4*1H-,1H+,4*1H-,1H+,4*1H-,
     2 1H+,4*1H-,1H+,4*1H-,1H+,4*1H-,1H+,4*1H-,1H+,4*1H-,1H+,4*1H-,1H+ /
      DATA SCALEH/10H                    1.0 +,4*10H                    ,10H      0.9 +,
     2 4*10H                    ,10H      0.8 +,4*10H                    ,10H      0.7 +,
     3 4*10H                    ,10H      0.6 +,2*10H                    ,10H (Z(K))2 ,
     4    10H                   ,10H      0.5 +,
     5 4*10H                    ,10H      0.4 +,4*10H                    ,10H      0.3 +,
     6 4*10H                    ,10H      0.2 +,4*10H                    ,10H      0.1 +,
     7 4*10H                    ,10H      0.0 +/
      DATA SCALEV /8H0.0      ,8H0.1      ,8H0.2      ,8H0.3      ,
     2 8H0.4      ,8H0.5      ,8H0.6      ,8H0.7      ,8H0.8      ,
     3 8H0.9      ,3H1.0/
      DATA SAMPLE / 8HZEROETH
     1              8HFIRST   ,8HSECOND  ,8HTHIRD   ,8HFOURTH  ,
     2              8HFIFTH   ,8HSIXTH   ,8HSEVENTH ,8HEIGHTH  ,
     3              8HNINTH   /
      DIMENSION BDRH(81)
      DATA BDRH/1H+,7*1H-,1H+,7*1H-,1H+,7*1H-,1H+,7*1H-,1H+,7*1H-,1H+,7*1H-,
     2 1H+,7*1H-,1H+,7*1H-,1H+,7*1H-,1H+,7*1H-,1H+,7*1H-,1H+,7*1H-,1H+/
      NL = 19
      NX = 80
      NY = 50
      NXP1 = NX + 1
      NYP1 = NY + 1
C     SET CONTOUR PLOT LIMITS
      XMIN = 0.
      XMAX = ZMAX
      YMIN = 0.
      YMAX = ZMAX
      DX = (XMAX - XMIN)/NX
      DY = (YMAX - YMIN)/NY
      NTTY = 59
      WRITE(NTTY,200))
 2001 FORMAT(*       NPLOT          KNS       IIMAX=)
      READ(NTTY,2002)NPLOT,KNS,IIMAX
 2002 FORMAT(3I10)
      READ(NIN)N,M,LL,NTL,TO,T1,LIMIT
      READ(NIN)((A(I,J),J=1,N),I=1,N)
      READ(NIN)((WKP1(I,J),J=1,N),I=1,N)
      READ(NIN)((WSS(I,J),J=1,N),I=1,N)
      READ(NIN)((CAPW(I,J),J=1,LL),I=1,LL)
      READ(NIN)((CAPV(I,J),J=1,M),I=1,M)
      IF(NTL.GT.0)READ(NIN)(((TITLES(I,J),J=1,8),I=1,NTL)
 3000 CONTINUE
      READ(NIN)NOP,T,ERRLIM,DT
      IF(NOP.LT.0) GO TO 99
      READ(NIN)((P(I,J),J=1,N),I=1,N)
      IF(NOP.GT.0)READ(NIN)(ZDUM(I),I=1,M)
      IF(NOP.GT.0)READ(NIN)(ZDUM(I),I=1,M)
      IF(NPLOT.EQ.0) GO TO 3001
      IF(NPLOT.GT.NOP) GO TO 3000
 3001 CONTINUE
      NOPP1 = NOP+1
      II = 0
    3 CONTINUE
      NS = KNS*II
      TP = T + NS*DT
      X(1) = XMIN
      X(2) = YMIN
      IF(II.EQ.0) CALL FVAL(X,FMIN)
      IF(II.GT.0) CALL PVAL(X,FMIN,NS)
      FMAX = FMIN
      DO 2 I=1,NYP1
C     X(1) HORIZONTALLY, X(2) VERTICALLY...
      X(2) = YMIN + (I-1)*DY
      DO 1 J=1,NXP1
```

```
      X(I) = XMIN + (J-1)*DX
      IF(I.EQ.0) CALL FVAL (X,F(I,J))
      IF (I.GT.0) CALL PVAL (X,F(I,J),NS)
      IF(F(I,J).LT.FMIN)FMIN = F(I,J)
      IF(F(I,J).GT.FMAX)FMAX = F(I,J)
    1 CONTINUE
    2 CONTINUE
      DF = (FMAX - FMIN)/NL
      WRITE(NOUT,101)TP,(TITLES(1,J),J=1,8),T,(TITLES(2,J),J=1,8),
     2                    NS,SAMPLE(NOPP1)
  101 FORMAT(*1*,10X,*CONTOUR PLOT OF TRACE(P(K,K+N)(Z(K))] AS *,
     1 *FUNCTION OF*
     2 * [Z(K)]1 HORIZ, [Z(K)]2 VERT*,9X,*T(K+N)=*,E11.4,/,
     3 11X,8A10,9X,*T(K)  =*,E11.4,/,11X,8A10,9X,*N = *,I3,
     4 * STEPS AFTER*,/,100X,A8,*MEASUREMENT*)
      WRITE(NOUT,107)BDRH
  107 FORMAT(10X,81A1,9X,16(1H=))
      DO 1000 I=1,NYP1
      DO 9 J=1,NXP1
      DO 5 K=1,NL
      IF(FMIN+K*DF).GT.F(NYP1+1-I,J))GO TO 6
    5 CONTINUE
    6 SLINE(J) = S(K)
      IF((F(NYP1+1-I,J)).EQ.FMIN) SLINE(J) = 1H=
      IF((F(NYP1+1-I,J)).EQ.FMAX) SLINE(J) = 1HO
    9 CONTINUE
      IF(I.GT.7)GO TO 280
      GO TO(21,22,23,24,25,26,27),I
   21 WRITE(NOUT,201)SCALEH(I),SLINE,BDR(I)
  201 FORMAT(A10,81A1,A1,6X,* CONTOUR LEVELS=)
      GO TO 1000
   22 WRITE(NOUT,202)SCALEH(I),SLINE,BDR(I)
  202 FORMAT(A10,81A1,A1,6X,*  AND SYMBOLS=)
      GO TO 1000
   23 WRITE(NOUT,203)SCALEH(I),SLINE,BDR(I)
  203 FORMAT(A10,81A1,A1,6X,16(1H=))
      GO TO 1000
   24 WRITE(NOUT,204)SCALEH(I),SLINE,BDR(I)
  204 FORMAT(A10,81A1,A1,6X,*SYMB LEVEL RANGE=)
      GO TO 1000
   25 WRITE(NOUT,203)SCALEH(I),SLINE,BDR(I)
      GO TO 1000
   26 WRITE(NOUT,206)SCALEH(I),SLINE,BDR(I),FMAX
  206 FORMAT(A10,81A1,A1,6X,4H (O),E11.4)
      GO TO 1000
   27 WRITE(NOUT,207)SCALEH(I),SLINE,BDR(I)
  207 FORMAT(A10,81A1,A1,6X,16(1H-))
      NSKIP = 1
      NLEVEL = 8
      GO TO 1000
  280 IF(I.GT.34)GO TO 350
      GO TO(28,28,29),NSKIP
   28 FLEVEL = FMIN + (2*NLEVEL+1-NSKIP)*DF
      WRITE(NOUT,208)SCALEH(I),SLINE,BDR(I),SYMB(NLEVEL),FLEVEL
  208 FORMAT(A10,81A1,A1,6X,* (*,A1,*)=*,E11.4)
      NSKIP = NSKIP+1
      GO TO 1000
   29 NSKIP = 1
      NLEVEL = NLEVEL - 1
      WRITE(NOUT,207)SCALEH(I),SLINE,BDR(I)
      GO TO 1000
  350 LINE = I - 34
      GO TO(35,36,37,38,39,40,36,42,43,44,45,36,47,48,44,50,51,52),LINE
   35 WRITE(NOUT,235)SCALEH(I),SLINE,BDR(I),FMIN
  235 FORMAT(A10,81A1,A1,6X,4H (*),E11.4)
      GO TO 1000
   36 WRITE(NOUT,203)SCALEH(I),SLINE,BDR(I)
      GO TO 1000
   37 WRITE(NOUT,237)SCALEH(I),SLINE,BDR(I)
  237 FORMAT(A10,81A1,A1,6X,*ESTIMATION=)
      GO TO 1000
   38 WRITE(NOUT,238)SCALEH(I),SLINE,BDR(I)
  238 FORMAT(A10,81A1,A1,6X,*ERROR CRITERION=)
      GO TO 1000
   39 WRITE(NOUT,239)SCALEH(I),SLINE,BDR(I)
  239 FORMAT(A10,81A1,A1,6X,*CONSTRAINT =*)
      GO TO 1000
   40 WRITE(NOUT,240)SCALEH(I),SLINE,BDR(I),ERRLIM
  240 FORMAT(A10,81A1,A1,12X,E11.4)
      GO TO 1000
   42 WRITE(NOUT,242)SCALEH(I),SLINE,BDR(I)
  242 FORMAT(A10,81A1,A1,6X,*SOURCE INPUT*)
      GO TO 1000
   43 WRITE(NOUT,243)SCALEH(I),SLINE,BDR(I)
  243 FORMAT(A10,81A1,A1,6X,*COVARIANCE  (W)=*)
      GO TO 1000
   44 WRITE(NOUT,244)SCALEH(I),SLINE,BDR(I)
  244 FORMAT(A10,81A1,A1)
      GO TO 1000
   45 WRITE(NOUT,245)SCALEH(I),SLINE,BDR(I),CAPW(1,1)
```

```
  245  FORMAT(A10,81A1,A1,8X,*[    *,E11.4,*]*)
       GO TO 1000
   47  WRITE(NOUT,247)SCALEH(I),SLINE,BDR(I)
  247  FORMAT(A10,81A1,A1,8X,*MEASUREMENT*)
       GO TO 1000
   48  WRITE(NOUT,248)SCALEH(I),SLINE,BDR(I)
  248  FORMAT(A10,81A1,A1,8X,*ERROR COVAR CV1=*)
       GO TO 1000
   50  WRITE(NOUT,250)SCALEH(I),SLINE,BDR(I),CAPV(1,1),CAPV(1,2)
  250  FORMAT(A10,81A1,A1,8X,*[*,F6.3,4X,F6.3,*]*)
       GO TO 1000
   51  WRITE(NOUT,250)SCALEH(I),SLINE,BDR(I),CAPV(2,1),CAPV(2,2)
       GO TO 1000
   52  WRITE(NOUT,203)SCALEH(I),SLINE,BDR(I)
 1000  CONTINUE
       WRITE(NOUT,107)BORH
       WRITE(NOUT,253)SCALEV
  253  FORMAT(/,9X,11A8,/,5IX,*[Z(K)]*)
       CALL MATOUT (P,N,N,1HP,NOUT,10)
       CALL EMPTY(NOUT)
       II = II + 1
       IF(II.LE.IIMAX) GO TO 3
       IF(NPLOT.EQ.0) GO TO 3000
   99  CALL EXIT
       END


       SUBROUTINE FVAL (Z,TRP)
       COMMON /PROB/ N,M,ZMAX,P,CAPV,ISING
       DIMENSION P(10,10),C(10,10),CAPV(10,10),PSI[(10,10)
       DIMENSION Z(1),W1(10,10),W2(10,10),W3(10,10)
       ND = 10
       PI = 3.14159266
       DO 12 I=1,M
       DO 11 J=1,N
   11  C(I,J) = COS((J-1)*PI*Z(I))
   12  CONTINUE
C      FIRST COMPUTE [PSI[] == [C*P(K-1,K)*CT]INVERSE...
       DO 5 IA=1,M
       DO 2 IC=1,N
       W1(IA,IC) = 0.
       DO 1 ID=1,N
    1  W1(IA,IC) = W1(IA,IC) + C(IA,ID)*P(ID,IC)
    2  CONTINUE
       DO 4 IB=1,M
       W2(IA,IB) = CAPV(IA,IB)
       DO 3 IE=1,N
    3  W2(IA,IB) = W2(IA,IB) + W1(IA,IE)*C(IB,IE)
    4  CONTINUE
    5  CONTINUE
       CALL INVERSE (M,W2,PSI[,IERR)
       IF(IERR.LT.0) GO TO 991
C      COMPUTATION OF TR[P(ZK)(K,K)]...
       TRP = 0.
       DO 10 IA=1,N
       TRP = TRP + P(IA,IA)
       DO 7 IC=1,M
       W1PI = 0.
       DO 6 ID=1,M
    6  W1PI = W1PI + W1(ID,IA)*PSI[(ID,IC)
    7  TRP = TRP - W1PI*W1(IC,IA)
   10  CONTINUE
       ISING = 0
   99  RETURN
  991  ISING = 3
       RETURN
       END


       SUBROUTINE PVAL (Z,TRP,NS)
C      CALCULATES TRACE(PIK,K+NS)), FOR (NS) TIME STEPS (DT) BEYOND (TIME
       COMMON /PROB/ N,M,ZMAX,P,CAPV,ISING
       COMMON /PROB2/ A,WKP1,DT,T
       DIMENSION P(10,10),CAPV(10,10),A(10,10),WKP1(10,10),Z(2)
       DIMENSION C(10,10),PSI[(10,10),PKP1(10,10)
       DIMENSION W1(10,10),W2(10,10),W3(10,10)
       PI = 3.14159266
C
C      FIRST, WITH THE VECTOR OF MEASUREMENT POSITIONS (Z), FIND THE
C      CORRECTED COVARIANCE MATRIX (W2) FROM THE LAST VALUE OF THE
C      PREDICTED COVARIANCE MATRIX (P) (IN COMMON) AT TIME (TIME)
C
       DO 12 I=1,M
       DO 11 J=1,N
   11  C(I,J) = COS((J-1)*PI*Z(I))
   12  CONTINUE
C
C      NEXT, COMPUTE [PSI[] == [C*P(K-1,K)*CT]INVERSE...
C
       DO 5 IA=1,M
```

```
267         DO 2 IC=1,N
268         W1(IA,IC) = 0.
269         DO 1 ID=1,N
270       1 W1(IA,IC) = W1(IA,IC) + C(IA,ID)*P(ID,IC)
271       2 CONTINUE
272         DO 4 IB=1,M
273         W2(IA,IB) = CAPV(IA,IB)
274         DO 3 IE=1,N
275       3 W2(IA,IB) = W2(IA,IB) + W1(IA,IE)*C(IB,IE)
276       4 CONTINUE
277       5 CONTINUE
278         CALL INVERSE (M,W2,PSI,,IERR)
279         IF(IERR.LT.0) GO TO 991
280 C
281 C       COMPUTE (P(K,K)) MATRIX, BUT FIND ONLY DIAGONAL ELEMENTS
282 C       TO BE USED TO INITIATE TRACE CALCULATION...
283 C
284         DO 10 IA=1,N
285         PKP1(IA,IA) = P(IA,IA)
286         DO 7 IC=1,M
287         W1P1 = 0.
288         DO 6 ID=1,M
289       6 W1P1 = W1P1 + W1(ID,IA)*PSI(ID,IC)
290       7 PKP1(IA,IA) = PKP1(IA,IA) - W1P1*W1(IC,IA)
291      10 CONTINUE
292 C
293 C       COMPUTATION OF TR(P(K,K+NS))...
294 C       PREDICT THE COVARIANCE MATRIX AHEAD (NS) STEPS IN TIME.
295 C       COMPUTE ONLY THE DIAGONAL ELEMENTS SINCE THE TRACE IS REQUIRED...
296 C
297         DO 16 K=1,NS
298         DO 15 I=1,N
299      15 PKP1(I,I) = A(I,I)*PKP1(I,I)*A(I,I) + WKP1(I,I)
300      16 CONTINUE
301         TRP = 0.
302         DO 17 I=1,N
303      17 TRP = TRP + PKP1(I,I)
304         ISING = 0
305      99 RETURN
306     991 ISING = 3
307         RETURN
308         END


309         SUBROUTINE MATOUTP (A,N,M,NAME,NOUT,ND)
310         DIMENSION A(ND,ND)
311         WRITE(NOUT,101)NAME
312     101 FORMAT(/,20X,A4,13H MATRIX IS...,/)
313         DO 1 I=1,N
314       1 WRITE(NOUT,102)(A(I,J),J=1,M)
315     102 FORMAT(20X,10E10.3)
316         RETURN
317         END


318         SUBROUTINE INVERSE (NN,A,AINV,IERROR)
319 C       SEE PROGRAM KALMAN FOR THIS ROUTINE...
320         END


321         SUBROUTINE DECOMP (NN,A,UL,SCALES,IPS,IERROR,ND)
322 C       SEE PROGRAM KALMAN FOR THIS ROUTINE...
323         END


324         SUBROUTINE SOLVE (NN,UL,B,X,IPS,ND)
325 C       SEE PROGRAM KALMAN FOR THIS ROUTINE...
326         END


327         SUBROUTINE IMPRUV (NN,A,UL,B,X,R,DX,IPS,DIGITS,IERROR,ND)
328 C       SEE PROGRAM KALMAN FOR THIS ROUTINE...
329         END
```

```
      PROGRAM PELEM (PFILE,TAPE2=PFILE,PEOUT,TAPE3=PEOUT)
C     SET (NPLOT) TO THE NUMBER OF THE MEASUREMENT FOR WHICH THE CONTOUR
C     PLOTS ARE DESIRED (1, 2,...).  SET IT TO ZERO (0) IF PLOTS
C     ARE DESIRED AFTER ALL MEASUREMENTS...
      CALL CREATE (8HPEOUT,40000,SWT)
      NIN = 2
      NOUT = 3
      NTTY = 59
      DIMENSION A(10,10),WKP1(10,10),CAPV(10,10),P(10,10)
      DIMENSION CAPW(10,10)
      DIMENSION WSS(10,10)
      DIMENSION ZDUM(10)
      ZMAX = 1.0
      COMMON /PROB/ N,M,ZMAX,P,CAPV,ISING
C
      DIMENSION F(51,81),X(2),S(19),SLINE(81),SYMB(9)
      DATA S / 1H ,1H1,1H ,1H2,1H ,1H3,1H ,1H4,1H ,1H5,
     2         1H ,1H6,1H ,1H7,1H ,1H8,1H ,1H9,1H  /
      DATA SYMB /1H1,1H2,1H3,1H4,1H5,1H6,1H7,1H8,1H9 /
      DIMENSION TITLES(4,8),BDR(51),SCALEH(81),SCALEV(11),SAMPLE(10)
      DATA BDR / 1H+,4*1H-,1H+,4*1H-,1H+,4*1H-,1H+,4*1H-,1H+,4*1H-,1H+,
     2 1H+,4*1H-,1H+,4*1H-,1H+,4*1H-,1H+,4*1H-,1H+,4*1H-,1H+ /
      DATA SCALEH/10H          1.0 ,4*10H                    ,10H      0.9 ,
     2 4*10H                    ,10H      0.8 ,4*10H                    ,10H      0.7 ,
     3 4*10H                    ,10H      0.6 ,2*10H                    ,10H (Z(K))2 .,
     4      10H                 ,10H      0.5 ,
     5 4*10H                    ,10H      0.4 ,4*10H                    ,10H      0.3 ,
     6 4*10H                    ,10H      0.2 ,4*10H                    ,10H      0.1 ,
     7 4*10H                    ,10H      0.0 /
      DATA SCALEV /8H0.0      ,8H0.1      ,8H0.2      ,8H0.3      ,
     2 8H0.4      ,8H0.5      ,8H0.6      ,8H0.7      ,8H0.8      ,
     3 8H0.9      ,3H1.0/
      DATA SAMPLE / 8HZEROETH
     1              8HFIRST   ,8HSECOND  ,8HTHIRD   ,8HFOURTH  ,
     2              8HFIFTH   ,8HSIXTH   ,8HSEVENTH ,8HEIGHTH  ,
     3              8HNINTH   /
      DIMENSION BDRH(81)
      DATA BDRH/1H+,7*1H-,1H+,7*1H-,1H+,7*1H-,1H+,7*1H-,1H+,7*1H-,1H+,
     2 1H+,7*1H-,1H+,7*1H-,1H+,7*1H-,1H+,7*1H-,1H+,7*1H-,1H+,7*1H-,1H+/
      NL = 19
      NX = 80
      NY = 50
      NXP1 = NX + 1
      NYP1 = NY + 1
C     SET CONTOUR PLOT LIMITS
      XMIN = 0.
      XMAX = ZMAX
      YMIN = 0.
      YMAX = ZMAX
      DX = (XMAX - XMIN)/NX
      DY = (YMAX - YMIN)/NY
      NTTY = 59
      WRITE(NTTY,2001)
2001  FORMAT(*    NPLOT=*)
      READ(NTTY,2002)NPLOT
2002  FORMAT(I10)
      READ(NIN)N,M,LL,NTL,TO,T1,LIMIT
      READ(NIN)((A(I,J),J=1,N),I=1,N)
      READ(NIN)((WKP1(I,J),J=1,N),I=1,N)
      READ(NIN)((WSS(I,J),J=1,N),I=1,N)
      READ(NIN)((CAPW(I,J),J=1,LL),I=1,LL)
      READ(NIN)((CAPV(I,J),J=1,M),I=1,M)
      IF(NTL.GT.0)READ(NIN)((TITLES(I,J),J=1,8),I=1,NTL)
3000  CONTINUE
      READ(NIN)NOP,T,ERRLIM,DT
      IF(NOP.LT.0) GO TO 99
      READ(NIN)((P(I,J),J=1,N),I=1,N)
      IF(NOP.GT.0)READ(NIN)(ZDUM(I),I=1,M)
      IF(NOP.GT.0)READ(NIN)(ZDUM(I),I=1,M)
      IF(NPLOT.EQ.0) GO TO 3001
      IF(NPLOT.GT.NOP) GO TO 3000
3001  CONTINUE
      NOPP1 = NOP+1
      II = 0
3     CONTINUE
      X(1) = XMIN
      X(2) = YMIN
      IF(II.EQ.0) CALL FVAL (X,FMIN)
      IF(II.GT.0) CALL PVAL(X,II,FMIN)
      FMAX = FMIN
      DO 2 I=1,NYP1
C     X(1) HORIZONTALLY, X(2) VERTICALLY...
      X(2) = YMIN + (I-1)*DY
      DO 1 J=1,NXP1
      X(1) = XMIN + (J-1)*DX
      IF(II.EQ.0) CALL FVAL (X,F(I,J))
      IF(II.GT.0) CALL PVAL(X,II,F(I,J))
      IF(F(I,J).LT.FMIN)FMIN = F(I,J)
      IF(F(I,J).GT.FMAX)FMAX = F(I,J)
1     CONTINUE
```

```
  2     CONTINUE
        DF = (FMAX - FMIN)/NL
        IF (I.EQ.0) WRITE (NOUT,100) T,(TITLES(1,J),J=1,8),SAMPLE(NOPP1),
       2 (TITLES(2,J),J=1,8)
  100  FORMAT(*1*,10X,*CONTOUR PLOT OF TRACE(P(K,K+N)(Z(K)))' AS *,
       1 *FUNCTION OF*
       2 * (Z(K))' HORIZ. (Z(K))2 VERT*,9X,*TIME=*,E11.4,/,
       3 11X,6A10,9X,A8 *MEASUREMENT*,/,11X,8A10,/)
        IF (I.GT.0) WRITE (NOUT,101) T,(TITLES(1,J),J=1,8),SAMPLE(NOPP1),
       2 (TITLES(2,J),J=1,8),II,II
  101  FORMAT(*1*,10X,*CONTOUR PLOT OF TRACE(P(K,K+N)(Z(K)))' AS *,
       1 *FUNCTION OF*
       2 * (Z(K))' HORIZ. (Z(K))2 VERT*,9X,*TIME=*,E11.4,/,
       3 11X,6A10,9X,A8,*MEASUREMENT*,/,11X,6A10,9X,
       4      *ELEMENT(*,I2,*,*,I2,*)*,/)
        WRITE(NOUT,107)BORH
  107  FORMAT(10X,81A1,9X,16(1H*))
        DO 1000 I=1,NYPI
        DO 9 J=1,NXP1
        DO 5 K=1,NL
        IF((FMIN+K*DF).GT.F(NYP1+1-I,J))GO TO 6
  5     CONTINUE
  6     SLINE(J) = S(K)
        IF((F(NYP1+1-I,J)).EQ.FMIN) SLINE(J) = 1H*
        IF((F(NYP1+1-I,J)).EQ.FMAX) SLINE(J) = 1HO
  9     CONTINUE
        IF(I.GT.7)GO TO 200
        GO TO(21,22,23,24,25,26,27),I
  21    WRITE(NOUT,201)SCALEH(I),SLINE,BOR(I)
  201   FORMAT(A10,81A1,A1,8X,* CONTOUR LEVELS=)
        GO TO 1000
  22    WRITE(NOUT,202)SCALEH(I),SLINE,BOR(I)
  202   FORMAT(A10,81A1,A1,8X,*  AND SYMBOLS=)
        GO TO 1000
  23    WRITE(NOUT,203)SCALEH(I),SLINE,BOR(I)
  203   FORMAT(A10,81A1,A1,8X,16(1H=))
        GO TO 1000
  24    WRITE(NOUT,204)SCALEH(I),SLINE,BOR(I)
  204   FORMAT(A10,81A1,A1,8X,*SYMB LEVEL RANGE=)
        GO TO 1000
  25    WRITE(NOUT,205)SCALEH(I),SLINE,BOR(I)
        GO TO 1000
  26    WRITE(NOUT,206)SCALEH(I),SLINE,BOR(I),FMAX
  206   FORMAT(A10,81A1,A1,8X,4H (0),E11.4)
        GO TO 1000
  27    WRITE(NOUT,207)SCALEH(I),SLINE,BOR(I)
  207   FORMAT(A10,81A1,A1,8X,16(1H-))
        NSKIP = 1
        NLEVEL = 9
        GO TO 1000
  200   IF(I.GT.34)GO TO 350
        GO TO(28,28,29),NSKIP
  28    FLEVEL = FMIN + (2+NLEVEL+1-NSKIP)*DF
        WRITE(NOUT,208)SCALEH(I),SLINE,BOR(I),SYMB(NLEVEL),FLEVEL
  208   FORMAT(A10,81A1,A1,8X,* (*,A1,*)=,E11.4)
        NSKIP = NSKIP+1
        GO TO 1000
  29    NSKIP = 1
        NLEVEL = NLEVEL - 1
        WRITE(NOUT,207)SCALEH(I),SLINE,BOR(I)
        GO TO 1000
  350   LINE = I - 34
        GO TO(35,36,37,38,39,40,36,42,43,44,45,35,47,48,44,50,51,52),LINE
  35    WRITE(NOUT,235)SCALEH(I),SLINE,BOR(I),FMIN
  235   FORMAT(A10,81A1,A1,8X,4H (*),E11.4)
        GO TO 1000
  36    WRITE(NOUT,203)SCALEH(I),SLINE,BOR(I)
        GO TO 1000
  37    WRITE(NOUT,237)SCALEH(I),SLINE,BOR(I)
  237   FORMAT(A10,81A1,A1,8X,*ESTIMATION=)
        GO TO 1000
  38    WRITE(NOUT,238)SCALEH(I),SLINE,BOR(I)
  238   FORMAT(A10,81A1,A1,8X,*ERROR CRITERION=)
        GO TO 1000
  39    WRITE(NOUT,239)SCALEH(I),SLINE,BOR(I)
  239   FORMAT(A10,81A1,A1,8X,*CONSTRAINT =*)
        GO TO 1000
  40    WRITE(NOUT,240)SCALEH(I),SLINE,BOR(I),ERRLIM
  240   FORMAT(A10,81A1,A1,12X,E11.4)
        GO TO 1000
  42    WRITE(NOUT,242)SCALEH(I),SLINE,BOR(I)
  242   FORMAT(A10,81A1,A1,8X,*SOURCE INPUT=)
        GO TO 1000
  43    WRITE(NOUT,243)SCALEH(I),SLINE,BOR(I)
  243   FORMAT(A10,81A1,A1,8X,*COVARIANCE   [W]=*)
        GO TO 1000
  44    WRITE(NOUT,244)SCALEH(I),SLINE,BOR(I)
  244   FORMAT(A10,81A1,A1)
        GO TO 1000
  45    WRITE(NOUT,245)SCALEH(I),SLINE,BOR(I),CAPW(I,1)
```

```
181   245  FORMAT(A10,81A1,A1,8X,*[    *,E11.4,*]*)
182        GO TO 1000
183   47   WRITE(NOUT,247)SCALEH(I),SLINE,BDR(I)
184   247  FORMAT(A10,81A1,A1,8X,*MEASUREMENT*)
185        GO TO 1000
186   48   WRITE(NOUT,248)SCALEH(I),SLINE,BDR(I)
187   248  FORMAT(A10,81A1,A1,8X,*ERROR COVAR [V]=*)
188        GO TO 1000
189   50   WRITE(NOUT,250)SCALEH(I),SLINE,BDR(I),CAPV(1,1),CAPV(1,2)
190   250  FORMAT(A10,81A1,A1,8X,*[*,F5.3,4X,F5.3,*]*)
191        GO TO 1000
192   51   WRITE(NOUT,250)SCALEH(I),SLINE,BDR(I),CAPV(2,1),CAPV(2,2)
193        GO TO 1000
194   52   WRITE(NOUT,203)SCALEH(I),SLINE,BDR(I)
195   1000 CONTINUE
196        WRITE(NOUT,107)BDRH
197        WRITE(NOUT,253)SCALEV
198   253  FORMAT(/,9X,11A0,/,51X,*[Z(K)]*)
199        CALL MATOUTP (P,N,N,IHP,NOUT,10)
200        CALL EMPTY(NOUT)
201        II = II + 1
202        IF(II.LE.N) GO TO 3
203        IF(NPLOT.EQ.0) GO TO 3000
204   99   CALL EXIT
205        END


206        SUBROUTINE FVAL (Z,TRP)
207   C    SEE PROGRAM NEWPT FOR THIS ROUTINE...
208        END


209        SUBROUTINE PVAL (Z,II,PII)
210   C    RETURNS (II,II)TH ELEMENT OF (P(K+1,K+1))...
211        COMMON /PROB/ N,M,ZMAX,P,CAPV,ISING
212        DIMENSION P(10,10),C(10,10),CAPV(10,10),PSI((10,10)
213        DIMENSION Z(1),W1((10,10),W2(10,10),W3(10,10)
214        ND = 10
215        PI = 3.14159265
216        DO 12 I=1,M
217        DO 11 J=1,N
218   11   C(I,J) = COS((J-1)*PI*Z(I))
219   12   CONTINUE
220   C    FIRST COMPUTE [PSI(] == [C*P(K-1,K)*CT]INVERSE...
221        DO 5 IA=1,M
222        DO 2 IC=1,N
223        W1((A,IC) = 0.
224        DO 1 ID=1,N
225   1    W1((A,IC) = W1((A,IC) + C((A,ID)*P((D,IC)
226   2    CONTINUE
227        DO 4 IB=1,M
228        W2((A,IB) = CAPV((A,IB)
229        DO 3 IE=1,N
230   3    W2((A,IB) = W2((A,IB) + W1((A,IE)*C((B,IE)
231   4    CONTINUE
232   5    CONTINUE
233        CALL INVERSE (M,W2,PSI(,IERR)
234        IF((IERR.LT.0) GO TO 991
235   C    CALCULATION OF [P(ZK)(K,K)]I(...
236        PII = P((I,II)
237        DO 7 IC=1,M
238        WIPI = 0.
239        DO 6 ID=1,M
240   6    WIPI = WIPI + W1((ID,II)*PSI((ID,IC)
241   7    PII = PII - WIPI*W1((C,II)
242        ISING = 0
243   99   RETURN
244   991  ISING = 3
245        RETURN
246        END


247        SUBROUTINE MATOUTP (A,N,M,NAME,NOUT,ND)
248        DIMENSION A(ND,ND)
249        WRITE(NOUT,101)NAME
250   101  FORMAT(/,20X,A4,13H MATRIX IS...,/)
251        DO 1 I=1,N
252   1    WRITE(NOUT,102)(A((,J),J=1,M)
253   102  FORMAT(20X,10E10.3)
254        RETURN
255        END


256        SUBROUTINE INVERSE (NN,A,AINV,IERROR)
257   C    SEE PROGRAM KALMAN FOR THIS ROUTINE...
258        END
```

```
      SUBROUTINE DECOMP (NN,A,UL,SCALES,IPS,IERROR,ND)
C     SEE PROGRAM KALMAN FOR THIS ROUTINE...
      END

      SUBROUTINE SOLVE (NN,UL,B,X,IPS,ND)
C     SEE PROGRAM KALMAN FOR THIS ROUTINE...
      END

      SUBROUTINE IMPRUV (NN,A,UL,B,X,R,DX,IPS,DIGITS,IERROR,ND)
C     SEE PROGRAM KALMAN FOR THIS ROUTINE...
      END
```

```
      PROGRAM SIGMAT (PFILE,TAPE2=PFILE,SOUT,TAPE3=SOUT)
      CALL CHANGE (2H+S)
      CALL CREATE (4HSOUT,40000,SWT)
      NIN = 2
      NOUT = 3
      DIMENSION SIGZ(101),Z(101)
      DIMENSION A(10,10),P(10,10),CAPV(10,10),WKP1(10,10),WSS(10,10)
      DIMENSION CAPW(10,10),ZDUM(10),TITLES(4,8)
      ND = 10
      COMMON /PROD/ N,M,ZMAX,A,P,CAPV,WKP1,WSS,ISING
      XNAME = 10HPOSITION Z
      YNAME = 10HSIG(Z,K+N)
      PNAME = 10HTIME TK+N
      ZMAX = 1.0
      XMIN = 0.0
      XMAX = ZMAX
      NX = 100
      NXP1 = NX+1
      DX = (XMAX-XMIN)/NX
      NTTY = 99
      WRITE(NTTY,1001)
 1001 FORMAT(=      NPLTS      NSKIP=)
      READ(NTTY,1002)NPLTS,NSKIP
 1002 FORMAT(2I10)
      READ(NIN)N,M,LL,NTL,TOL,TIMLIT
      READ(NIN)((A(I,J),J=1,N),I=1,N)
      READ(NIN)((WKP1(I,J),J=1,N),I=1,N)
      READ(NIN)((WSS(I,J),J=1,N),I=1,N)
      READ(NIN)((CAPW(I,J),J=1,LL),I=1,LL)
      READ(NIN)((CAPV(I,J),J=1,M),I=1,M)
      IF(NTL.GT.0)READ(NIN)((TITLES(I,J),J=1,8),I=1,NTL)
    5 CONTINUE
      READ(NIN)NOP,T,ERRLIM,DT
      IF(NOP.LT.0) GO TO 99
      READ(NIN)((P(I,J),J=1,N),I=1,N)
      IF(NOP.GT.0)READ(NIN)(ZDUM(I),I=1,M)
      IF(NOP.GT.0)READ(NIN)(ZDUM(I),I=1,M)
      FMIN = SIGMA (0.)
      FMAX = FMIN
      DO 3 II=1,NPLTS
      PVALUE = T + (II-1)*DT*NSKIP
      DO 1 I=1,NXP1
      Z(I) = XMIN + (I-1)*DX
      SIGZ(I) = SIGMA(Z(I))
    1 CONTINUE
      CALL MULTPLT (Z,SIGZ,II,XNAME,YNAME,PNAME,PVALUE,TITLES,NTL,NOUT)
      DO 2 K=1,NSKIP
    2 CALL APATW (A,P,WKP1,N,ND)
    3 CONTINUE
      II = -1
      CALL MULTPLT (Z,SIGZ,II,XNAME,YNAME,PNAME,PVALUE,TITLES,NTL,NOUT)
      GO TO 5
   99 CONTINUE
      PVALUE = (WSS(1,1)/WKP1(1,1))*DT
      YNAME = 10HS GMA(WSS)
      PNAME = 10HTIME TO SS
      DO 101 I=1,N
      DO 100 J=1,N
  100 P(I,J) = WSS(I,J)
  101 CONTINUE
C     ZERO OUT FIRST ELEMENT OF (WSS)...
      P(1,1) = 0.0
      DO 102 I=1,NXP1
      Z(I) = XMIN + (I-1)*DX
      SIGZ(I) = SIGMA(Z(I))
  102 CONTINUE
      II = 1
      CALL MULTPLT (Z,SIGZ,II,XNAME,YNAME,PNAME,PVALUE,TITLES,NTL,NOUT)
      II = -1
      CALL MULTPLT (Z,SIGZ,II,XNAME,YNAME,PNAME,PVALUE,TITLES,NTL,NOUT)
      CALL EXIT
      END

      FUNCTION SIGMA(Z)
C     SEE PROGRAM KALMAN FOR THIS ROUTINE...
      END

      SUBROUTINE XTAY (X,A,Y,Q,N,ND)
C     SEE PROGRAM KALMAN FOR THIS ROUTINE...
      END

      SUBROUTINE APATW (A,P,W,N,ND)
      DIMENSION A(10,10),P(10,10),W(10,10)
      DO 2 I=1,N
      DO 1 J=1,N
    1 P(I,J) = A(I,I)*P(I,J)*A(J,J) + W(I,J)
    2 CONTINUE
```

```
      RETURN
      END

      SUBROUTINE MULTPLT (XIN,YIN,N,XNAME,YNAME,PNAME,PVALUE,
     2 TITLES,NTL,NOUT)
      DIMENSION XIN(101),YIN(101),X(1010),Y(1010),PARAM(10)
      DIMENSION TITLES(4,8)
      MAXPTS = 101
      IF(N.LT.0) GO TO 90
      NUMPTS = N*MAXPTS
      NPLTS = N
      PARAM(N) = PVALUE
      DO 1 I=1,MAXPTS
      II = (N-1)*MAXPTS + I
      X(II) = XIN(I)
      Y(II) = YIN(I)
1     CONTINUE
      RETURN
90    CONTINUE
      CALL PARALST (X,Y,NPLTS,NUMPTS,XNAME,YNAME,PNAME,PARAM,
     2 TITLES,NTL,NOUT)
      CALL PARAPLT (X,Y,NPLTS,NUMPTS,XNAME,YNAME,PNAME,PARAM,
     2 TITLES,NTL,NOUT)
      RETURN
      END

      SUBROUTINE PARALST (X,Y,NPLTS,NUMPTS,XNAME,YNAME,PNAME,PARAM,
     2 TITLES,NTL,NOUT)
      DIMENSION X(1010),Y(1010),PARAM(10),SYMBOL(10),EQUALS(11),TERM(11)
      DIMENSION TITLES(4,8)
      DATA EQUALS / 11*1OH==========/
      DATA SYMBOL / 1HO,1H1,1H2,1H3,1H4,1H5,1H6,1H7,1H8,1H9/
      IF(NTL.EQ.0) GO TO 2
      DO 1 I=1,NTL
1     WRITE(NOUT,101)(TITLES(I,J),J=1,8)
101   FORMAT(1X,8A10)
2     WRITE(NOUT,102)PNAME,(PARAM(I),I=1,NPLTS)
102   FORMAT(/,* TABULAR LIST OF PLOTTED PARAMETRIC CURVES*,//,
     2 A10,10(1X,E10.3))
      NPLTSP1 = NPLTS+1
      WRITE(NOUT,104)(EQUALS(I),I=1,NPLTSP1)
104   FORMAT(A10,10(1X,A10))
      WRITE(NOUT,103)(SYMBOL(I),I=1,NPLTS)
103   FORMAT(*POSITION 2 *,10(*SIG(2,K+* A1,*) *))
      WRITE(NOUT,104)(EQUALS(I),I=1,NPLTSP1)
      DO 5 I=1,101
      TERM(I) = X(I)
      DO 4 J=1,NPLTS
4     TERM(J+1) = Y((J-1)*101+I)
5     WRITE(NOUT,106)(TERM(K),K=1,NPLTSP1)
106   FORMAT(E10.3,10(1X,E10.3))
      RETURN
      END

      SUBROUTINE PARAPLT (X,Y,NPLTS,NUMPTS,XNAME,YNAME,PNAME,PARAM,
     2 TITLES,NTL,NOUT)
      DIMENSION X(1010),Y(1010),S(1010),PARAM(10)
      DIMENSION SYMBOL(10)
      DIMENSION TITLES(4,8)
      DIMENSION POINTS(101),BUT(6)
      DIMENSION SST(1010)
      DATA SST /101*1HO,101*1H1,101*1H2,101*1H3,101*1H4,101*1H5,
     2 101*1H6,101*1H7,101*1H8,101*1H9 /
      DATA SYMBOL /1HO,1H1,1H2,1H3,1H4,1H5,1H6,1H7,1H8,1H9/
      DO 1 I=1,NUMPTS
1     S(I) = SST(I)
      IF(NUMPTS.LT.2)GO TO 999
C WRITE OUT TITLE CARDS
      WRITE(NOUT,6)
6     FORMAT(1H1)
      DO 3 I=1,4
      GO TO (301,302,302,302),I
301   IF(I.LE.NTL) WRITE(NOUT,2001)YNAME,(TITLES(I,J),J=1,8)
2001  FORMAT(3X,A10,2X,8A10)
      IF(I.GT.NTL) WRITE(NOUT,2002)YNAME
2002  FORMAT(3X,A10)
      GO TO 3
302   IF(I.LE.NTL)WRITE(NOUT,2003)(TITLES(I,J),J=1,8)
2003  FORMAT(15X,8A10)
      IF(I.GT.NTL) WRITE(NOUT,5)
3     CONTINUE
      WRITE(NOUT,5)
5     FORMAT(1H )
C
C RE-ORDER BY THE Y AXIS.
C
C SOLVE FOR MAX
```

```
      I=1
20    CONTINUE
      JJ=I
      YMAX=Y(I)
      DO 10 J=I,NUMPTS
      IF(Y(J).LE.YMAX)GO TO 10
      YMAX=Y(J)
      JJ=J
10    CONTINUE
C INTERCHANGE
      YY=Y(I)
      XX=X(I)
      SS = S(I)
      Y(I)=Y(JJ)
      X(I)=X(JJ)
      S(I) = S(JJ)
      Y(JJ)=YY
      X(JJ)=XX
      S(JJ) = SS
      I=I+1
      IF(I.EQ.NUMPTS)GO TO 30
      GO TO 20
30    CONTINUE
C SOLVE FOR MIN/MAX OF X AND Y.
      XMIN=X(1)
      XMAX=X(1)
      YMIN=Y(1)
      YMAX=Y(1)
      DO 2 I=1,NUMPTS
      IF(X(I).LT.XMIN)XMIN=X(I)
      IF(X(I).GT.XMAX)XMAX=X(I)
      IF(Y(I).LT.YMIN)YMIN=Y(I)
      IF(Y(I).GT.YMAX)YMAX=Y(I)
2     CONTINUE
C RESET THE END POINTS.
      CALL ENDPTS(XMIN,XMAX)
      CALL ENDPTS(YMIN,YMAX)
C CALCULATE DELX AND DELY.
      DELX=(XMAX-XMIN)/100.0
      DELY=(YMAX-YMIN)/50.0
C GENERATE THE PLOT
      KK=ABS(XMIN)/DELX+1.0
      IZERO=0
      IF((XMIN.LE.0.0).AND.(XMAX.GE.0.0))IZERO=1
      ICOUNT=10
      LIST=1
      DO 100 I=1,51
      XI=I
      YZ2=YMAX-XI*DELY
      YZ1=YZ2+DELY
      IAA=0
      IF((YZ1.GE.0.0).AND.(YZ2.LE.0.0))IAA=1
      DO 101 J=1,101
101   POINTS(J)=1H
      IF(ICOUNT.NE.10)GO TO 105
      DO 106 J=1,101,2
106   POINTS(J)=1H.
105   CONTINUE
      POINTS(  1)=1H.
      POINTS( 21)=1H.
      POINTS( 41)=1H.
      POINTS( 61)=1H.
      POINTS( 81)=1H.
      POINTS(101)=1H.
      IF(IZERO.EQ.1)POINTS(KK)=1H|
      IF(IAA.NE.1)GO TO 137
      DO 136 J=1,101
136   POINTS(J)=1H-
137   CONTINUE
      YLOW=YMAX-XI*DELY
102   CONTINUE
      IF(LIST.GT.NUMPTS)GO TO 110
      IF(Y(LIST).LT.YLOW)GO TO 110
      K=(X(LIST)-XMIN)/DELX+1.0
      POINTS(K) = S(LIST)
      LIST=LIST+1
      GO TO 102
110   CONTINUE
      IF(ICOUNT.EQ.10)GO TO 112
      ICOUNT=ICOUNT+1
      WRITE(NOUT,111)(POINTS(J),J=1,101)
111   FORMAT(15X,101A1)
      GO TO 100
112   CONTINUE
      YY=YLOW+DELY
      ICOUNT=1
      IF((YY.GT.-1.0E-9).AND.(YY.LT.1.0E-9))YY=0.0
      WRITE(NOUT,113)YY,(POINTS(J),J=1,101)
113   FORMAT(2X,E11.4,2X,101A1)
100   CONTINUE
```

```
      DO 121 I=1,6
      XI=I-1
      BUT(I)=XMIN+20.0*DELX*XI
      IF((BUT(I).LT.1.0E-9).AND.(BUT(I).GT.-1.0E-9))BUT(I)=0.0
121   CONTINUE
      WRITE(NOUT,122)(BUT(J),J=1,6)
122   FORMAT(/,10X,6(E10.3,10X))
      WRITE(NOUT,2004)XNAME
2004  FORMAT(61X,A10)
      WRITE(NOUT,3000)PNAME,((SYMBOL(I),PARAM(I)),I=1,NPLTS)
3000  FORMAT(*1*,////,1X,18(**=*),/,*  PARAMETER VALUE*,/,
     2 *     AND SYMBOL*,/,1X,18(**=*),/,*  SYMB   =*,A10,/,1X,18(*-=*),/,
     3 10(*    (*,A1,*) =*,E11.4,/))
      WRITE(NOUT,6)
999   CONTINUE
      RETURN
      END

      SUBROUTINE ENDPTS(XMIN,XMAX)
C     SEE PROGRAM KALMAN FOR THIS ROUTINE...
      END
```

```
      PROGRAM MAXTIME (PFILE,TAPE2=PFILE,MOUT,TAPE3=MOUT)
      CALL CHANGE (5H+MAXT)
      CALL CREATE (4HMOUT,10000,SWT)
      NIN = 2
      NOUT = 3
      ND = 10
      DIMENSION A(10,10),P(10,10),CAPV(10,10),WKP1(10,10),WSS(10,10),
     2          CAPW(10,10),CAPMO(10,10),TIME(110),TRP(110),PP(10,10),
     3          ZST(10,2,10),TITLES(4,8)
      READ(NIN)N,M,LL,NTL,TO,T1,LIMIT
      READ(NIN)((A(I,J),J=1,N),I=1,N)
      READ(NIN)((WKP1(I,J),J=1,N),I=1,N)
      READ(NIN)((WSS(I,J),J=1,N),I=1,N)
      READ(NIN)((CAPW(I,J),J=1,LL),I=1,LL)
      READ(NIN)((CAPV(I,J),J=1,M),I=1,M)
      IF(NTL.GT.0) READ(NIN)((TITLES(I,J),J=1,8),I=1,NTL)
      READ(NIN)NOP,T,ERRLIM,DT
      READ(NIN)((CAPMO(I,J),J=1,N),I=1,N)
    3 CONTINUE
      READ(NIN)NOP,T,ERRLIM,DT
      IF(NOP.LT.0) GO TO 4
      READ(NIN)((P(I,J),J=1,N),I=1,N)
      READ(NIN)(ZST(I,2,NOP),I=1,M)
      READ(NIN)(ZST(I,1,NOP),I=1,M)
C     NOTE...ORDER OF STORAGE OF OPTIMAL ZK-VECTORS IS REVERSED, THAT I
C     ZK* FOR TRACE INDEX COMES OUT OF KALMAN FIRST, BUT IS STORED
C     IN ZST(I,2,NOP), WHEREAS ZK* FOR P11 INDEX COMES OUT SECOND
C     AND IS STORED IN ZST(I,1,NOP).  ALL THIS TO PLOT PUU, THEN TRACE I
C     BUT IS STORED IN ZST(I,1,NOP).
C     ALL THIS IN ORDER TO PLOT P11 FIRST, THEN TRACE, HERE.
      GO TO 3
    4 CONTINUE
      DO 50 II=1,2
      IF(II.EQ.1) WRITE(NOUT,102)
  102 FORMAT(*1*,/ * CRITERION NUMBER 1, PLOTTED WITH SYMBOL (1).*,/,
     2 * MINIMIZE [P(K,K+N)]11 WITH RESPECT TO Z(K).*,//,
     3 *            K                  T          TRP*,/)
      IF(II.EQ.2) WRITE(NOUT,103)
  103 FORMAT(*1*,/ * CRITERION NUMBER 2, PLOTTED WITH SYMBOL (2).*,/,
     2 * MINIMIZE TRACE[P(K,K+N)] WITH RESPECT TO Z(K).*,//,
     3 *            K                  T          TRP*,/)
      NOP = 0
      CALL ATOB(CAPMO,P,N,N,ND)
      CALL ATOB(CAPMO,PP,N,N,ND)
      T = TO
      K = 1
   20 CONTINUE
      TEST = TR(PP,N)
      IF(TEST.GE.ERRLIM) GO TO 28
      TIME(K) = T
      TRP(K) = TEST
      WRITE(NOUT,101)K,T,TEST
  101 FORMAT(I10,2E10.3)
      IF(T.GT.T1) GO TO 45
      IF(K.EQ.110) GO TO 45
      T = T + DT
      K = K + 1
      CALL ATOB (PP,P,N,N,ND)
      CALL PREDICT (A,P,WKP1,PP,N,ND)
      GO TO 20
   28 CONTINUE
      IF(K.GT.1) T = T - DT
      NOP = NOP + 1
      CALL CORRECT(ZST(1,II,NOP),P,CAPV,PP,ISING,N,M,ND)
      GO TO 20
   45 CONTINUE
      XII = II
      CALL MULTPLT (TIME,TRP,II,K,10HTIME TK+N ,10HTRP(K,K+N),
     2 10H CRITERION,XII,TITLES,NTL,NOUT)
   50 CONTINUE
      II = -1
      CALL MULTPLT (TIME,TRP,II,K,10HTIME TK+N ,10HTRP(K,K+N),
     2 10H CRITERION,XII,TITLES,NTL,NOUT)
      CALL EXIT
      END


      SUBROUTINE PREDICT (A,P,W,PP,N,ND)
      DIMENSION A(10,10),P(10,10),W(10,10),PP(10,10)
C     PERFORMS THE ONE-STEP PREDICTION...
C     PP = (A*P*A-TRANSPOSE) + W
C     WHERE A IS A DIAGONAL STATE TRANSITION MATRIX
      DO 2 I=1,N
      DO 1 J=1,N
    1 PP(I,J) = A(I,I)*P(I,J)*A(J,J) + W(I,J)
    2 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE CORRECT(Z,P,CAPV,PP,ISING,N,M,ND)
      DIMENSION P(10,10),C(10,10),CAPV(10,10),PSI(10,10),PP(10,10)
      DIMENSION Z(1),W1(10,10),W2(10,10),W3(10,10)
      PI = 3.14159266
      DO 12 I=1,M
      DO 11 J=1,N
   11 C(I,J) = COS((J-1)*PI*Z(I))
   12 CONTINUE
C     FIRST COMPUTE [PSI] == [C*P(K-1,K)*CT]INVERSE...
      DO 5 IA=1,M
      DO 2 IC=1,N
      W1(IA,IC) = 0.
      DO 1 ID=1,N
    1 W1(IA,IC) = W1(IA,IC) + C(IA,ID)*P(ID,IC)
    2 CONTINUE
      DO 4 IB=1,M
      W2(IA,IB) = CAPV(IA,IB)
      DO 3 IE=1,N
    3 W2(IA,IB) = W2(IA,IB) + W1(IA,IE)*C(IB,IE)
    4 CONTINUE
    5 CONTINUE
      CALL INVERSE (M,W2,PSI(),IERR)
      IF(IERR.LT.0) GO TO 991
C     COMPUTE FULL (P(ZK)(K,K)) MATRIX...
      DO 10 IA=1,N
      DO 7 IC=1,M
      W3(IA,IC) = 0.
      DO 6 ID=1,M
    6 W3(IA,IC) = W3(IA,IC) + W1(ID,IA)*PSI(ID,IC)
    7 CONTINUE
      DO 9 IB=1,N
      W2(IA,IB) = P(IA,IB)
      DO 8 IE=1,M
    8 W2(IA,IB) = W2(IA,IB) - W3(IA,IE)*W1(IE,IB)
      PP(IA,IB) = W2(IA,IB)
    9 CONTINUE
   10 CONTINUE
      ISING = 0
   99 RETURN
  991 ISING = 3
      RETURN
      END

      SUBROUTINE ATOB  (A,B,N,M,ND)
C     SEE PROGRAM KALMAN FOR THIS ROUTINE...
      END

      FUNCTION TR(A,N)
C     SEE PROGRAM KALMAN FOR THIS ROUTINE...
      END

      SUBROUTINE INVERSE (NN,A,AINV,IERROR)
C     SEE PROGRAM KALMAN FOR THIS ROUTINE...
      END

      SUBROUTINE DECOMP (NN,A,UL,SCALES,IPS,IERROR,ND)
C     SEE PROGRAM KALMAN FOR THIS ROUTINE...
      END

      SUBROUTINE SOLVE (NN,UL,B,X,IPS,ND)
C     SEE PROGRAM KALMAN FOR THIS ROUTINE...
      END

      SUBROUTINE IMPROV (NN,A,UL,B,X,R,DX,IPS,DIGITS,IERROR,ND)
C     SEE PROGRAM KALMAN FOR THIS ROUTINE...
      END

      SUBROUTINE MULTPLT (XIN,YIN,N,NPTS,XNAME,YNAME,PNAME,PVALUE,
     2 TITLES,NTL,NOUT)
C     SEE PROGRAM SIGMAT FOR THIS ROUTINE...
      END

      SUBROUTINE PARAPLT(X,Y,NPLTS,NUMPTS,NEACH,XNAME,YNAME,PNAME,PARAM
     2 TITLES,NTL,NOUT)
C     SEE PROGRAM SIGMAT FOR THIS ROUTINE...
      END

      SUBROUTINE ENDPTS(XMIN,XMAX)
C     SEE PROGRAM KALMAN FOR THIS ROUTINE...
      END
```

```
      PROGRAM POSTPLT (TFILE,TAPE2=TFILE,PPOUT,TAPE3=PPOUT)
      CALL CHANGE (3H+PP)
      CALL CREATE (5HPPOUT,10000,SWT)
      NIN = 2
      NOUT = 3
      DIMENSION YNAME(2),PNAME(2)
      DATA YNAME / 10HTRACK,K+N),10HSIG(K,K+N) /
      DATA PNAME / 10HTRACELIM  ,10HSIGMALIM   /
      DIMENSION TIME(110),XT(110),TITLES(4,8)
      II = 1
1     CONTINUE
      READ(NIN)N,M,LL,NTL,T0,T1,LIMIT,ERRLIM
      IF(N.LT.0) GO TO 50
      IF(NTL.GT.0)READ(NIN)((TITLES(I,J),J=1,8),I=1,NTL)
      READ(NIN)NPTS
      READ(NIN)(TIME(I),I=1,NPTS)
      READ(NIN)(XT(I),I=1,NPTS)
      WRITE(NOUT,101)YNAME(LIMIT),II,PNAME(LIMIT),ERRLIM,YNAME(LIMIT)
101   FORMAT(*1*,/,* PLOT OF *,A10,* VERSUS TIME, PLOTTED WITH SYMBOL *,
     2 I1,/,* ESTIMATION ERROR LIMIT *,A10,* = *,E10.3,//,
     3 *          TIME*,A10,//)
      DO 2 I=1,NPTS
2     WRITE(NOUT,102)TIME(I),XT(I)
102   FORMAT(2E10.3)
      CALL MULTPLT (TIME,XT,II,NPTS,10HTIME TK+N,
     2 YNAME(LIMIT),PNAME(LIMIT),ERRLIM,TITLES,NTL,NOUT)
      II = II + 1
      GO TO 1
50    II = -1
      CALL MULTPLT (TIME,XT,II,NPTS,10HTIME TK+N,
     2 YNAME(LIMIT),PNAME(LIMIT),ERRLIM,TITLES,NTL,NOUT)
      CALL EXIT
      END

      SUBROUTINE MULTPLT (XIN,YIN,N,NPTS,XNAME,YNAME,PNAME,PVALUE,
C     SEE PROGRAM SIGMAT FOR THIS ROUTINE...
      END

      SUBROUTINE PARAPLT(X,Y,NPLTS,NUMPTS,NEACH,XNAME,YNAME,PNAME,PARAM,
C     SEE PROGRAM SIGMAT FOR THIS ROUTINE...
      END

      SUBROUTINE ENDPTS(XMIN,XMAX)
C     SEE PROGRAM KALMAN FOR THIS ROUTINE...
      END
```

```
      PROGRAM POSTFP (PFILE,TAPE2=PFILE,FPOUT,TAPE3=FPOUT)
      CALL CHANGE (3H*FP)
      CALL CREATE (6HFPOUT,10000,SWT)
      DIMENSION Z(10),X(110),FX(110)
      COMMON /PROB/ N,M,ZMAX,A,P,CAPV,WKP1,WSS,ISING
      DIMENSION A(10,10),P(10,10),CAPV(10,10),WKP1(10,10),WSS(10,10)
      DIMENSION CAPW(10,10)
      DIMENSION TITLES(4,8)
      NIN = 2
      NOUT = 3
      NTTY = 59
      YNAME = 10HP(K,K)]11
      PNAME = 10HDIMENS. NS
      DZ = 0.01
      ZMAX = 1.0
    1 WRITE(NTTY,1001)
 1001 FORMAT(*[Z(K)]2=*)
      READ(NTTY,1002)Z(2)
 1002 FORMAT(E10.3)
      IF(Z(2).LT.0) GO TO 99
      REWIND NIN
      II = 1
 3000 CONTINUE
      READ(NIN)N,M,LL,NTL,TO,T1,LIMIT
      IF(N.LT.0) GO TO 50
      READ(NIN)((A(I,J),J=1,N),I=1,N)
      READ(NIN)((WKP1(I,J),J=1,N),I=1,N)
      READ(NIN)((WSS(I,J),J=1,N),I=1,N)
      READ(NIN)((CAPW(I,J),J=1,LL),I=1,LL)
      READ(NIN)((CAPV(I,J),J=1,M),I=1,M)
      IF(NTL.GT.0)READ(NIN)((TITLES(I,J),J=1,8),I=1,NTL)
      READ(NIN)NOP,T,ERRLIM,DT
      READ(NIN)((P(I,J),J=1,N),I=1,N)
      DO 5 I=1,101
      Z(1) = (I-1)*DZ
      X(I) = Z(1)
      CALL FVAL(Z,FX(I))
    5 CONTINUE
      WRITE(NOUT,101)Z(2),N,N
  101  FORMAT(*1*,/,* PLOT OF [P(K,K)]11 FOR [Z(K)]2 = *,E10.3,/,
     2 * VERSUS POSITION [Z(K)]1 FOR MODEL DIMENSION NS = *,I2,/,
     3 * PLOTTED WITH SYMBOL (*,I1,*)*,//,
     4 *[Z(K)]1    [P(K,K)]11*,//)
      CALL MULTPLT (X,FX,II,101,10H[Z(K)]1
     2 YNAME,PNAME,Z(2),TITLES,NTL,NOUT)
      II = II + 1
      GO TO 3000
   50 CONTINUE
      CALL MULTPLT (X,FX,II,101,10H[Z(K)]1
     2 YNAME,PNAME,Z(2),TITLES,NTL,NOUT)
      GO TO 1
   99 CALL EXIT
      END

      SUBROUTINE MULTPLT (XIN,YIN,N,NPTS,XNAME,YNAME,PNAME,PVALUE,
     2 TITLES,NTL,NOUT)
C     SEE PROGRAM SIGMAT FOR THIS ROUTINE...
      END

      SUBROUTINE PARAPLT(X,Y,NPLTS,NUMPTS,NEACH,XNAME,YNAME,PNAME,PARAM,
C     SEE PROGRAM SIGMAT FOR THIS ROUTINE...
      END

      SUBROUTINE ENDPTS(XMIN,XMAX)
C     SEE PROGRAM KALMAN FOR THIS ROUTINE...
      END

      SUBROUTINE FVAL (Z,P11)
C     SEE PROGRAM KALMAN FOR THIS ROUTINE...
      END

      SUBROUTINE INVERSE (NP,A,AINV,IERROR)
C     SEE PROGRAM KALMAN FOR THIS ROUTINE...
      END

      SUBROUTINE DECOMP (NN,A,UL,SCALES,IPS,IERROR,ND)
C     SEE PROGRAM KALMAN FOR THIS ROUTINE...
      END

      SUBROUTINE SOLVE (NN,UL,B,X,IPS,ND)
C     SEE PROGRAM KALMAN FOR THIS ROUTINE...
      END

      SUBROUTINE IMPROV (NN,A,UL,B,X,R,DX,IPS,DIGITS,IERROR,ND)
C     SEE PROGRAM KALMAN FOR THIS ROUTINE...
      END
```

```
      PROGRAM POSTSP (PFILE,TAPE2=PFILE,SPOUT,TAPE3=SPOUT)
      CALL CHANGL (3H+SP)
      CALL CREATE (5HSPOUT,10000,SWT)
      DIMENSION Z(10),X(110),FX(110),PDUM(10,10),XDUM(10)
      COMMON /PROB/ N,M,ZMAX,A,P,CAPV,WKP1,WSS,ISING
      DIMENSION A(10,10),P(10,10),CAPV(10,10),WKP1(10,10),WSS(10,10)
      DIMENSION CAPW(10,10)
      DIMENSION TITLES(4,8)
      NIN = 2
      NOUT = 3
      YNAME = 10HSIGMA2(Z)
      PNAME = 10HDIMENS. NS
      DZ = 0.01
      ZMAX = 1.0
    1 CONTINUE
      REWIND NIN
      II = 1
 3000 CONTINUE
      READ(NIN)N,M,LL,NTL,TO,T1,LIMIT
      IF(N.LT.0) GO TO 50
      READ(NIN)((A(I,J),J=1,N),I=1,N)
      READ(NIN)((WKP1(I,J),J=1,N),I=1,N)
      READ(NIN)((WSS(I,J),J=1,N),I=1,N)
      READ(NIN)((CAPW(I,J),J=1,LL),I=1,LL)
      READ(NIN)((CAPV(I,J),J=1,M),I=1,M)
      IF(NTL.GT.0)READ(NIN)((TITLES(I,J),J=1,8),I=1,NTL)
      READ(NIN)NOP,T,ERRLIM,DT
      READ(NIN)((PDUM(I,J),J=1,N),I=1,N)
      READ(NIN)NOP,T,ERRLIM,DT
      READ(NIN)((P(I,J),J=1,N),I=1,N)
      READ(NIN)(XDUM(I),I=1,M)
      READ(NIN)(XDUM(I),I=1,M)
    3 CONTINUE
      READ(NIN)NOP,T,ERRLIM,DT
      IF(NOP.LT.0) GO TO 4
      READ(NIN)((PDUM(I,J),J=1,N),I=1,N)
      READ(NIN)(XDUM(I),I=1,M)
      READ(NIN)(XDUM(I),I=1,M)
      GOTO 3
    4 CONTINUE
      DO 5 I=1,101
      Z(1) = (I-1)*DZ
      X(I) = Z(I)
      FX(I) = SIGMA(Z(1))
    5 CONTINUE
      CALL MULTPLT (X,FX,II,101,10HIZ(K)))
     2 YNAME,PNAME,Z(2),TITLES,NTL,NOUT)
      II = II + 1
      GO TO 3000
   50 CONTINUE
      WRITE(NOUT,101)N,N
  101 FORMAT(*1*,/,* PLOT OF SIGMA**2(Z)*,/,
     2 * VERSUS POSITION Z FOR MODEL DIMENSION NS = *,I2,/,
     3 * PLOTTED WITH SYMBOL (*,II,*)*)
      II = -1
      CALL MULTPLT (X,FX,II,101,10HIZ(K)))
     2 YNAME,PNAME,Z(2),TITLES,NTL,NOUT)
      CALL EMPTY(NOUT)
   99 CALL EXIT
      END

      FUNCTION SIGMA(Z)
C     SEE PROGRAM SIGMAT FOR THIS ROUTINE...
      END

      SUBROUTINE XTAY (X,A,Y,Q,N,ND)
C     SEE PROGRAM SIGMAT FOR THIS ROUTINE...
      END

      SUBROUTINE MULTPLT (XIN,YIN,N,NPTS,XNAME,YNAME,PNAME,PVALUE,
C     SEE PROGRAM SIGMAT FOR THIS ROUTINE...
      END

      SUBROUTINE PARAPLT(X,Y,NPLTS,NUMPTS,NEACH,XNAME,YNAME,PNAME,PARAM,
     2 TITLES,NTL,NOUT)
C     SEE PROGRAM SIGMAT FOR THIS ROUTINE...
      END

      SUBROUTINE ENDPTS(XMIN,XMAX)
C     SEE PROGRAM KALMAN FOR THIS ROUTINE...
      END
```

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